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CeRTEV - Center for Research, Technology and Education in Vitreous Materials

Report July 2020 – June 2021, FAPESP grant #2013/007796-3

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RESEARCH PROGRESS

1. Introduction and overview.

The **Ce**nter of **R**esearch, **T**echnology, and **E**ducation in **V**itreous Materials (CeRTEV) was founded with resources from the Research Foundation of the State of São Paulo to advance fundamental research and technological development in the area of glass and glass-ceramic science. It comprises 10 principal investigators, 4 permanent collaborators and their co-workers at the Federal University of São Carlos (UFSCar), the University of São Paulo (USP), (both located in São Carlos) and the State University of São Paulo (UNESP, Araraquara), located at 30 km from São Carlos. The principal investigators heading these groups are experts in vitreous materials, in their crystallization towards glass-ceramics, and in a wide range of structural and functional characterization techniques. They advise about 60 graduate students and post-docs engaging in glass and glass-ceramic research, and are embedded in a large Brazilian and international collaboration network. As part of the joint CeRTEV research agenda, these groups work together to develop new active glasses and glass-ceramics, presenting application-relevant functionalities such as high mechanical strength, electrical conductivity, biological, optical or catalytic activity, and/or combinations of these properties.

Developing a glassy material with promising physical properties into an application-relevant functional device involves a process of multi-parameter optimization. For this objective, glasses are the perfect materials base: we can modify the physical properties of a glass over wide regions by adjusting its chemical composition, by adding new constituents and even by changing the way they are being made and processed after their synthesis. Thus, glasses offer a vast parameter space for ***fine-tuning*** a solid material for its desired application. Previously, much of this work had to be done empirically, by trial and error (***melting and testing***) which is costly, time-consuming, and obviously extremely inefficient. During the past few years, the ultimate goal of predicting the perfect glass composition for a given application, has been coming within reach. Three key developments are responsible for this paradigm shift: (1) results from 60 years of modern fundamental research on glasses have been organized in two comprehensive databases (SciGlass and Interglad), (2) highly effective algorithms have been developed for mining this database, then training and testing composition-property models via Machine Learning techniques, and (3) powerful theory-based and computational techniques allow the prediction of structures and properties from molecular dynamics simulations, and also from density functional theory. With this enormously powerful arsenal available for the simulation driven design of novel glasses for desired applications, we are currently entering an exciting and challenging decade of research and innovation.

On the side of knowledge-driven fundamental research we attack cutting–edge

fundamental research questions dealing with the thermodynamic and kinetic foundations of glass formation, relaxation, and crystallization towards glass-ceramics. We want to ***understand*** and predict ***glass-forming ability***, and how and why crystallization is suppressed upon cooling. We want to learn how to ***control*** the ***degree of crystallinity and the microstructure of glass-ceramics***. Exercising such control is of utmost importance for realizing desired physical-chemical properties such as ***high fracture strength and hardness*** (for impact resistant glasses), ***maximum ionic conductivity*** (for more high-power density batteries), and ***bioactive response*** (for osteo-inductive glassy scaffolds optimally adapted in their physiological environment).
On the side of application-oriented research we use our insights on composition-structure-property relationships to develop new and improved glasses and glass-ceramics for five principal high-end technology application areas: (1) ***structural reinforcement materials*** for architecture and construction, glasses with higher scratch- and impact resistance for TV and smartphone displays, for armor (*bullet-proof windows*), as well as for dental restoration, (2) ***bioactive glasses and glass-ceramics*** for implants (*spare body parts*) and to serve as scaffolds stimulating bone growth and tissue healing, (3) ***fast glass-ceramic ion-conductive materials*** enabling the design of lithium and sodium ion batteries with higher capacities and higher power-densities as required for electro motion, and (4) ***photonic glasses and glass-ceramics*** for high-power lasers and signal transmission conduits, for white-light emission, for high energy (UV, x-ray) radiation detection, electroluminescent devices and a plethora of chemo- and biosensor applications. During the 2020-2021 funding period, the CeRTEV investigators published approximately 60 articles dealing with fundamental and applied issues on glasses and glass-ceramics. These include review articles on fundamental issues, such as glass characterization, structure-property relations studied by advanced spectroscopic techniques, and various timely application fields as detailed below.

2. Fundamental research issues and progress.

2.1. Glass property predictions

Glass-forming ability (GFA) is a property of utmost importance in glass science and technology. In the search for suitable predictors, a statistical methodology was applied to develop reliable criteria based on the various characteristic temperatures published for a wide range of glass compositions: glass transition temperature (T_g), the onset of crystallization temperature (T_x), the temperature of the crystallization peak (T_g) and the liquidus temperature, (T_L). The Weinberg parameter $K_w = (T_c - T_g)/T_L$ was found to hold the strongest predictive power of glass-forming ability, which is related to the glass stability (GS) against crystallization [1]. The work, already discussed in the previous report, has now been published.
Against this theoretical background, an extensive experimental study was carried out to assess the influence of alkali and alkaline earth modifiers and five glass-formers, in the crystallization resistance of binary oxide glasses [2]. For the good glass formers silica, boria and germania, the addition of small amounts of modifiers rapidly reduces GS, whereas for the conditional glass formers telluria and alumina, it initially increases the GS. Lower liquidus temperatures are associated with a better GS, and above 50 mol% of modifier oxide, the liquidus temperature seems to be the main factor controlling GS (except for TeO_2). Lithium-containing glasses show the lowest GS between the alkali systems, while the alkaline earth modifiers show the same effect on the GS. The pure

oxides rank in the following order of GS: B_2O_3>SiO_2>GeO_2>TeO_2>Al_2O_3.
To move forward from (educated) trial-and-error to data- and simulation-driven strategies, a computer program was developed that combines data-driven predictive models (in this case, neural networks) with a genetic algorithm to design glass compositions with desired combinations of properties. Our studies considered the combination of a low glass transition temperature (T_g < 500 °C) and high refractive index (n_d > 1.7) using more than 40.000 datasets with 38 different chemical elements. Two candidate compositions suggested by the combined algorithms were selected and produced in the laboratory, yielding excellent results [3]. Our results are an important stepping stone in the pathway of machine learning-guided design of novel glasses.

2.2. Relaxation, Nucleation and Crystallization

Work during the past report period has focused on the role of liquid-phase separation [4], seeding [5], and structural relaxation in the nucleation process [6]. In particular, knowledge of structural relaxation processes is fundamental in glass science and technology because relaxation is intrinsically related to vitrification, annealing effects and the associated evolution of the physical properties of glasses. It can be monitored by measuring the temporal evolution of the refractive index, n_d, variation at temperatures between 5 and 25 K below the fictive temperature. There are conflicting reports in the literature on whether the structural relaxation time of glass can be calculated using the Maxwell equation, which relates relaxation time with shear viscosity and shear modulus. In an experimental study on lead metasilicate glass the experimental average structural relaxation times deduced from n_d measurements were found to be less than one order of magnitude higher than the average relaxation time computed through the Maxwell equation. Thus, the equilibrium shear viscosity only provides a lower boundary for structural relaxation kinetics [6]. This result is consistent with recent MD simulations on the glass former barium sulfide [7].
The failure of the Classical Nucleation Theory (CNT) to describe the temperature dependence of the homogeneous crystal nucleation rates below the temperature of maximum nucleation, T_{max}, has been pointed out frequently. In further on-going work, possible explanations for this suspected breakdown have been tested [8,9]. While the form and the results of the numerical solution of the set of kinetic equations describing nucleation are not affected by self-consistency corrections, neglecting the latter overestimates the work of critical cluster formation and leads, consequently, to far too low theoretical values for the steady-state nucleation rates [9].
In the application of the CNT and all other theoretical models of crystallization of liquids and glasses it is always assumed that nucleation proceeds only <u>after</u> the supercooled liquid or the glass have completed structural relaxation processes towards the metastable equilibrium state. As shown by both experimental data recently obtained on lithium disilicate glass [10] and new MD simulations on BaS [7] this condition may not necessarily be fulfilled. For situations where nucleation proceeds concomitantly with structural relaxation, new kinetic expressions were derived [11], taking into consideration adequate expressions for the thermodynamic driving force and the surface tension accounting for the contributions caused by the deviation of the supercooled liquid from metastable equilibrium. When the characteristic times of structural relaxation are of similar order of magnitude or longer than the characteristic times of crystal nucleation, elastic stresses evolving in nucleation may significantly affect this process. These results are relevant for the understanding of the breakdown of the

CNT referred to above, as discussed in a model study on soda-lime-silica glass [12].
Finally, we point out that, to the present date, the vast majority of fundamental studies on glass crystallization have been carried out using stoichiometric compositions. On the other hand, by far the most common cases in glass-ceramics technology are off-stoichiometric. In this context, recent experimental data have been discussed in terms of the CNT within a comprehensive study on the nucleation and growth kinetics of combeite crystals in non-stoichiometric glasses of the combeite (Na_2O•$2CaO$•$3SiO_2$) – devitrite (Na_2O•$3CaO$•$6SiO_2$) system [13].
On the experimental side, *in-situ* Raman spectroscopy has proven to be a powerful tool for elucidating crystallization mechanisms.[14]. Our most recent contribution in this vein has been the transformation of lead metasilicate glass into alamosite glass-ceramic, which may (depending on annealing protocols) involve the formation of two distinct metastable $PbSiO_3$ modifications. Substantial work has also been completed with the homogeneously nucleating barium disilicate composition. The crystallization mechanism is found to be profoundly influenced by temperature and pressure, suggesting that the melt structure is highly sensitive to these parameters [15]. A detailed theoretical analysis of the vibrational modes in Sanbornite (low-$BaSi_2O_4$) and $Ba_5Si_8S_{21}$ indicates that the vibrational frequencies are highly sensitive towards crystal chemical parameters, in particular Ba-O and Si-O bond lengths. These findings suggest that in-situ Raman spectroscopy may become a powerful tool for monitoring subtle local environment changes reflecting structural relaxation and nucleation processes that occur upon annealing [16].

3. Strong glasses and glass-ceramics

Work during the 2020/2021 funding period includes the development of new formulations and functionalities as well as contributions towards a further fundamental understanding of their properties on a structural basis.
Certain strong glasses and glass-ceramics have found widespread use in dentistry due to their favorable properties: biocompatibility, chemical inertness, high fracture strength and toughness, superior esthetics, color stability, and translucence. A lithium metasilicate (LS) glass-ceramic was developed showing a house-of-cards microstructure composed of 50% vol. plate-like LS crystals of 5–25 µm, randomly dispersed in a glassy matrix [17]. Lithium disilicate (12% vol.), two minor crystal phases, and 34% vol. residual glass was also present. Its physical characteristics are the following: fracture toughness 3.5 ± 0.5 MPa $m^{1/2}$, fracture strength 450 ± 40 MPa. The elastic modulus 124 ± 2 GPa, the linear thermal expansion coefficient 13.6×10^{-6} °C^{-1}. Its solubility in 4%vol. acetic acid (215 ± 30 µg/cm^2) is well below the limit established by the ISO 6872 standard for some applications, but not suitable for uncoated use. The further optimization of these properties is subject to ongoing study.
Transparent and translucent glass-ceramics (GCs) are found in an increasing number of domestic and high-technology applications. Using two-stage annealing, a new highly crystalline glass ceramic (52% $Li_2Si_2O_5$ 26% Li_2SiO_3) having a transmittance of 80% visible light through 1.2 mm thick specimens was developed in the SiO_2–Li_2O–P_2O_5–TiO_2–CaO–ZnO–Al_2O_3 system [18], Its physical characteristics are: nano-hardness 8.7 ± 0.1 GPa (load of 400 mN), elastic modulus 138 ± 3 GPa, and flexural strength (350 ± 40 MPa). Applications of this material for displays of electronic devices are currently under consideration. In similar work, femtosecond laser pulses were used to inscribe optical waveguides inside a magnesium aluminum silicate (MAS) precursor glass and glass-

ceramic [19], which has shown satisfactory mechanical properties to be applied as ballistic armor. Its good optical waveguiding and mechanical properties indicate that this new TGC might be adequate for photonic devices that require high mechanical strength. Another important glass design challenge in the field of ultra-strong glasses has been to negotiate the inherent tradeoff between crack initiation resistance (CR) and elastic modulus (E). In borosilicate glasses these properties principally depend on the average coordination number of the boron atoms, leading to an inverse correlation of CR and E. It is possible, however, to accommodate the conflicting demands of high CR and E values, by using magnesium oxide in the glass formulation. This effect has been explored in a series of aluminoborosilicate glasses with the compositions $60SiO_2$-$10Al_2O_3$-$10B_2O_3$-(20-x)Na_2O-xRO and $60SiO_2$-$10Al_2O_3$-$10B_2O_3$-(20-x)RO-xR'O (R,R' = Mg,Ca,Sr,Ba) [18]. This systematic study points towards a decisive effect of the average ionic potential $\xi = Ze/r$ of the network modifier cations. on both (CR) and E. Systematic trends indicating an increase of CR with increasing ionic potential, ξ, have been correlated with structural properties deduced from the NMR interaction parameters in ^{29}Si, ^{27}Al, ^{23}Na, and ^{11}B solid state NMR [20].

4. Bioactive Glasses

4.1. New functionalities and application fields

During the current review period the application potential of the two principal bioactive glass formulations previously developed at CeRTEV, which are biosilicate (BS) and F18, was further explored for applications in dental restoration, osteo-stimulation, and tissue engineering.

New conical implants based on the Biosilicate formulation were successfully tested for anophthalmic socket reconstruction [21], with good results suggesting that. this implant may provide a good alternative to the only conical implant currently available on the market, which is composed of porous polyethylene. Biosilicate was also successfully tested for various dental applications. As an additive to H_2O_2 -containing bleaching gels, it reduces the extent of pulp damage induced by dental bleaching [22]. As an ingredient in tricalcium silicate dental cements it enhances the antimicrobial properties of the latter [23]. In an effort of improving the bioactivity of biosilicate for bone repair, collagen from marine spongin (SPG) has been used as a promising material for tissue engineering proposals. Accordingly, (SPG)-enriched BS composites were tested, using a critical experimental model of cranial bone defect in rats. Supported by histopathological and immunohistochemistry analyses, this *in-vivo* study demonstrates that the BS and BS/SPG scaffolds are biocompatible and able to support bone formation in a critical bone defect in rats [24]. Similarly, photobiomodulation (PBM) treatment applied in conjunction was shown to be effective in modulating inflammatory processes after an injury, accelerating soft and hard tissue healing and stimulating neoangiogenesis [25]. These results suggest that the combined SPG/BS and PBM treatment procedure may have therapeutic prospects. The favorable gene expression profile of the human adipose-derived stem cells (hASCs) grown on the Biosilicate®/F18 glass (BioS-2P/F18) scaffolds was characterized [26]. After 14 days, the gene expression of different proteins involved in osteoblast differentiation was significantly up-regulated in hASCs grown on the scaffolds, as compared to hASCs cultured with the ionic extract of the osteogenic medium. These results indicate that both the composition and topographic features of the biomaterial could stimulate osteogenesis [26].

Highly porous biosilicate foams were produced, to be used as scaffolds for bone tissue engineering [27]. To this end a gel-casting process was developed, based on the room temperature foaming of powders suspended in a "weakly alkaline" (1 M NaOH) aqueous solution, followed by sintering at 1,000°C. The homogeneity of foamed samples was assessed using micro-tomography and was further improved by casting foamed suspensions ("foam casting") before setting. Amorphous powders provided more intense gelation than semicrystalline ones, promoted a more homogeneous foaming, and stimulated a substantial extent of crystallization upon firing. Also, both direct ink writing and digital light processing techniques could be easily applied to fine powders of Biosilicate® mixed with fugitive binders for manufacturing highly porous scaffolds (porosity of 50–80 vol%) [28]. Significant densification of the struts, despite the limited powder packing, could be achieved using liquid-assisted sintering, already at 1,000 °C. The strength-to-density ratio could be flexibly tuned (from 1.5 to 9.5 MPa cm^3/g), especially with DLP-derived samples, by adjusting both the firing temperature and the scaffold topology.

F18 is a bioactive glass recently developed by CeRTEV researchers, which due to its outstanding GS, presents a much wider range of processing conditions when compared to other bioactive glasses, a feature that allows it to be used for coating metallic implants, sintering scaffolds, or manufacturing fibers for wound healing applications. Its bactericidal and anti-biofilm activity were investigated *in vitro* as a powder and as a coating on steel samples, and the effects of its dissolution products at concentrations from 3 mg/mL to 50 mg/mL against the *Staphylococcus aureus* and methicillin-resistant *Staphylococcus aureus* (MRSA) biofilms were explored. Indeed, F18 presents bactericidal activity in preformed *S. aureus* and MRSA biofilms, reducing the counts of the viable cells that remained in contact with 50 mg/mL for 24 h by six orders of magnitude. Moreover, an anti-biofilm activity was observed after 12 h of direct contact, with a similar drop in the viable bacterial population. Neutralization of the F18 solution pH decreases its bactericidal efficacy. These results indicate that F18 glass could be considered as an alternative material for controlling and treating infections by *S. aureus* [29].

A comparative *in-vivo* evaluation was done of the biocompatibility, induction of mineralization and antimicrobial activity of experimental intracanal pastes based on biosilicate (BS) and F18. Both were found to be biocompatible, stimulated biomineralization and induced significant osteopontin immunolabeling compared to a $Ca(OH)_2$ control sample. However, only the BS paste demonstrated antimicrobial activity comparable to $Ca(OH)_2$ [30]. F18 was further evaluated with respect to its ability of suppressing biofilm formation when applied as a coating on Ti surfaces. [31, 32]. While there was no clear inhibitory effect on biofilm growth, F18 was found to promote the modulation of virulence factors [33].

4.2. Composition/Structure/Property Correlations in Bioactive Glasses and Glass-Ceramics

Bioactive glasses and glass-ceramics (GCs) effectively regenerate bone tissue, however most GCs show improved mechanical properties. This was tested on a rarely studied potassium analogue of the 45S5 composition ($24.4K_2O$-$26.9CaO$-$46.1SiO_2$-$2.6P_2O_5$ mol%) with different particle sizes and heating rates to obtain a sintered GC that combines good fracture strength, low elastic modulus, and bioactivity. We analyzed the influence of the sintering processing conditions in the elastic modulus, Vickers microhardness, density, and crystal phase formation in the GC. The best GC shows

improved properties compared with its parent glass. This glass achieves a good densification degree with a two-step viscous flow sintering approach and the resulting GC shows as high bioactivity as that of the standard 45S5 Bioglass®. Furthermore, the GC elastic modulus (56 GPa) is relatively low, minimizing stress shielding [34]. The study was further extended to mixed sodium-potassium containing glasses based on the 45S5 formulation. The replacement of half of the Na_2O by K_2O significantly improves both the densification rate and the *in-vitro* performance, documenting the suitability of these glasses for the design of new bioactive materials with improved sinterability [35].
The glass stability of boron-containing bioglasses can be increased by incorporation of TiO_2. This effect was correlated with structural data in a series of glasses along the section (26 − 0.25x)CaO (26 − 0.25x)SrO (4 − 0.05x)B_2O_3-xTiO_2 (44 − 0.45x) SiO_2 ($0 \leq x \leq 8$) [36]. While the ^{11}B and ^{29}Si NMR spectra show little variation, they are consistent with Ti acting as a network modifier in this system [36]. Finally, a fundamental study, combining multinuclear advanced NMR methods, MD simulations, and DFT calculations based on GIPAW and PAW algorithms, was conducted to study the structural modification caused by incorporating small amounts (1 – 5 mole %) of P_2O_5 into perboric, metaboric and peralkaline sodium borosilicate glasses [37]. P_2O_5 preferentially attracts the network modifier species, thus resulting in a repolymerization of the silicate network and a restructuring of the borate component. $^{11}B\{^{31}P\}$ and $^{31}P\{^{11}B\}$ dipolar recoupling experiments suggest that the ability of glasses to incorporate P_2O_5 without phase separation is related to the formation of P-O-B(IV) linkages integrated into the borosilicate glass network. An analogous approach is used for elucidating the local environments of the Na^+ network modifiers. This work lays the foundation for the development of quantitative structure-property relationship (QSPR) models in bioactive borosilicate glasses, thus representing a leap forward in the design of glasses with controllable ionic release behavior.

5. Fast solid electrolyte glasses and glass-ceramics

Ion conducting glass-ceramics have shown significant promise for applications as solid electrolytes in high energy storage devices. The highest cationic mobilities in the solid state are generally encountered in crystalline compounds with highly disordered cation sub-lattices, termed *superionic crystals*. Nevertheless, ion conducting glasses have the advantage of not suffering from grain boundary effects and hence form more homogeneous interfaces with the anode and cathode compartments of a solid-state electrochemical cell. Thus, dense glass-ceramics based on the crystallization of suitable precursor glasses offer the promise of combining both favorable features. The CeRTEV research agenda focuses on the further development of such systems, based on a solid understanding of composition – structure – performance relationships. In particular, non-linear compositional dependences observed in such studies such as network-former mixing effects and mixed cation effects are subject of fundamental research aiming at the development of structural hypotheses.

5.1 Glass-ceramics based on the NASICON structure.

The development of new and improved glass-ceramics based on the NASICON structure has been a long-standing topic in CeRTEV's research agenda. Our most recent efforts in this area aim at the optimization of materials with longer-term sustainability. Motivated by the much larger natural abundance of the element sodium in comparison to lithium we are now focusing on the development of sodium-based compositions. Currently we are therefore exploring phase relations and ionic conductivity/structure relations of glass-ceramics generated from aliovalent substitution of the framework constituents in sodium titanium phosphate, $NaTi_2(PO_4)_3$, NTP, and sodium germanium phosphate, $NaGe_2(PO_4)_3$, NGP. During the past reporting period our efforts focused on optimizing the one- and two-step annealing protocols of the ceramization for maximizing ion transport [38]. In addition, a promising new composition, $Na_{3.4}Al_xSc_{2-x}Si_{0.4}P_{2.6}O_{12}$ ($0.0 \leq x \leq 1.7$) was developed and characterized. The Al^{3+}/Sc^{3+} isovalent substitution allows for variations in the lattice parameters without varying the number of charge carriers (Na^+ ions) per unit formula, impacting the ionic conductivity of the material [39].

5.2. Network former mixing and mixed cation effects in ion-conducting glasses.
Network former mixing effects on ionic conductivities were examined in the glass systems $(A_2O)_{0.3}$-$[(TeO_2)_x$-$(GeO_2)_{1-x}]_{0.7}$ (A = Li, Na, $0 \leq x \leq 1$). While the Li-based system displays a subtle positive effect detectable by both electrical conductivity measurements and static ^{7}Li NMR spectra, no such effect could be noticed in the Na-based system. The structural aspects of this effect were investigated by solid-state NMR and Raman spectroscopies [40]. While the fraction of four-coordinated Te species increases with increasing Te content in both systems, no clear evidence for hetero-atomic Te-O-Ge connectivity could be established in either of them. It appears that the relatively weak interaction between the two network formers GeO_2 and TeO_2 does not create energetically favorable target sites for the alkaline metal ions.
Multinuclear NMR measurements were further conducted to investigate mixed cation effects in the ternary Sr-Li-Cs metaphosphate glass system. The results reveal monotonic compositional evolutions of ^{31}P, ^{7}Li, and ^{133}Cs chemical shifts and ^{7}Li-^{7}Li, as well as ^{7}Li/^{133}Cs dipole-dipole coupling strengths, consistent with a random cation mixing model and the absence of any segregation or phase separation effects [41].

6. Photonic glasses and glass-ceramics
The design and photophysical characterization of highly efficient luminescent glasses and glass-ceramics for photonic devices is at the core of the CeRTEV research agenda. These systems are based on luminescent rare-earth (RE) ions, which must be well-dispersed within low-phonon environments, for most applications, to minimize non-radiative de-excitation of emitting levels. The properties of these materials can be enhanced and modified by the presence of metallic or semiconducting nanoclusters and –particles through plasmon resonance enhancement. Besides focusing on the development of optimized compositions for detection or high energy radiation (UV and X-ray) and near-infrared thermometry, research of the 2020/2021 funding period also included novel design strategies to obtain nanocomposites bearing RE and metallic/semiconductor nanoparticles, and the characterization of their functional properties. A new area to CeRTEV has been work on strongly paramagnetic glasses with intriguing magneto-optical properties. Structure-property correlations have been sought on the basis of a comprehensive spectroscopic strategy, based on the combination of NMR, EPR, Raman, optical absorption and emission spectroscopies.

6.1. New rare-earth doped glass and glass-ceramics formulations.
A variety of new, promising glass and glass-ceramic formulations were developed and their optical, luminescent and structural properties were analyzed as detailed below: They include,

(a) Radioluminescent fluorophosphate glasses with compositions 35$NaPO_3$-30$Ba(PO_3)_2$-25MgF_2-(10- x)YF_3–x[EuF_3 or Dy_2O_3] with x = 0–4.0 mol% EuF_3, or x = 0–1.0 mol% Dy_2O_3,for scintillator applications, that is conversion of high energy into visible light [42],

(b) Bismuth-containing rare-earth co-doped fluoride phosphate glasses for super-broadband near-infrared (NIR) emission with potential applications in optical amplification. Detailed NMR studies reveal a new network modification scheme involving depolymerization of polyphosphate chains under the formation of F-bonded fluorophosphate units. In addition, a significant part of the fluoride stays separate, interacting exclusively with metal-ion species [43].

(c) Lead and barium oxyfluoroborate glasses and glass-ceramics featuring RE doped fluorite nanocrystals upon crystallization [44]

(d) Calcium boroaluminate (CaBAl) glasses with composition (30.97-x)CaO-49.90B_2O_3-10.22Al_2O_3-8.90CaF_2-xCeO_2 for applications in white LEDs and phosphors [45],

(e) Triply-Rare-earth doped zinc-tellurite glasses for white-light generation. Tunable blue to cold-white light emission can be achieved via up-conversion under 980 nm, while adjusting the laser excitation intensity. The energy transfer properties and spectroscopic parameters were analyzed on the basis of Judd-Ofelt theory [46].

(f) Eu^{3+}-doped phosphate glasses and glass-ceramics with high tantalum oxide contents for photonic applications of non-linear optical properties. The precursor glass exhibits high photoluminescence quantum efficiency due to low phonon energy and high refractive index (1.9461 at 633 nm). Transparent $Na_2Ta_8O_{21}$ nanocrystals are formed in the glass-ceramic, nucleated at 925 °C for 0.5 h and grown at 940 °C for different times [47].

(g) Glass-ceramics based on Er^{3+} and Tm^{3+}-doped $Yb_3Ga_5O_{12}$ crystals prepared from controlled cooling of heavy-metal oxide glass melts. The RE cations are incorporated into the crystalline phase and display intense upconversion emissions of Er^{3+} (550 and 660 nm) and Tm^{3+} (800 nm) when pumped at 980 nm [48].

6.2. Glass/nanoparticle nanocomposites.

The incorporation of metallic nanoclusters (NCs) and nanoparticles (NPs) into glass matrices has led to a new family of mechanically stable nanocomposites that preserve the integrity (and hence the physical properties) of the nanocrystals, enabling application in photonics, catalysis, and chemical sensing. Significant work done during the current review period has been devoted to new nanocomposite formulations and the characterization of their optical properties. Various different strategies for the preparation of such nanocomposites were developed at CeRTEV and its partner laboratories. For example, traditional melt cooling/annealing procedures were used to prepare borosilicate glass samples singly- and co-doped with Er^{3+} and ZnSe nanoparticles in the quantum confinement regime. Intensity depleted regions at 377 and 521 nm observed in the excitation band of ZnSe indicate absorption by Er^{3+}due to energy transfer from the ZnSe NPs to Er^{3+} ions. Upon excitation at 367, 447 and 498 nm, ZnSe doped glasses give broad emission bands centered around 696 nm [49].

Alternatively, the sol-gel route has been employed as well for preparing homogeneous CdTe quantum dot/Er^{3+}-co-doped SiO_2–Nb_2O_5-based nanocomposites. These materials present tunable fluorescence in the range of 513–568 nm, depending on the particle sizes realized. Potential applications include devices for broadband emission, optical amplification and lighting [50]. A new study on the development of composite materials based on the inclusion of micro- and nanopowders exhibiting the persistent luminescence phenomenon, in glassy hosts has also been introduced. The dispersion of CoPt metallic nanoparticles within a glass-forming phosphate melt at 1000 °C for 15 minutes has also been successful, provided that the particles are protected by a dense silica layer in a prior preparation step [51]. Finally, a new direct laser writing approach has been used to prepare highly fluorescent silver clusters in a Eu^{3+}-doped silver-containing zinc phosphate glass. The observed significant enhancement of the fluorescence emission of the Eu^{3+} ions in the vicinity of UV-excited laser-inscribed silver clusters demonstrates the ability to perform efficient resonant non-radiative energy transfer from excited silver clusters to Eu^{3+}, allowing such energy transfer to be highly localized on demand, as controlled by laser inscription. These results open the route to 3D printing of the rare earth ions emission in glass [52].

6.3. Magneto-optic glasses

Strongly paramagnetic glasses prepared by incorporation of high concentrations of rare earth oxides have recently moved into the research focus because of their potential use as Faraday rotators. At CeRTEV, we have prepared various new magneto-optic glasses exploiting the high solubility of Gd_2O_3 and Tb_4O_7 in the borogermanate glass formulation (100-x) ($60GeO_2$-$25B_2O_3$-$4Al_2O_3$-$10Na_2O$-1PbO)– x RE_2O_3[53, 54]. The materials were systematically characterized with respect to their structural (XRD, EXAFS, XANES and Raman), thermal (DSC), morphological, optical, magnetic and magneto-optical (MO) properties. For Tb_4O_7-containing glasses, magnetic susceptibilities and Verdet constants increase proportionally to rare earth content, reaching -83.9 rad $T^{-1}m^{-1}$ at 650 nm for glass containing 8 mol% of Tb_4O_7. The optical window covers the range from 0.5 up to 1.6 µm. XANES and EXAFS measurements at the Ge-K edge show that the germanium atoms are tetrahedrally coordinated, while results at the Tb-LIII edge show terbium atoms to be eight-coordinated and exclusively present in the oxidation state 3+, independently of the glass composition. Good thermal stability (ΔT = 200 °C) allowed obtaining an optical fiber of a glass containing 4 mol% of Tb_4O_7 featuring Verdet constants of -37.9, -23.6 and -5.89 rad T^{-1} m^{-1}, at 500, 650 and 1550 nm, respectively [54]. The structural aspects of the mixed-network former base glass system (85-x)GeO_2-(x)B_2O_3-$10Na_2O$-$4Al_2O_3$-1PbO were examined by solid state NMR, while systematically varying the GeO_2/B_2O_3 ratio. The results provide insight into the competition of the three network former species Al, Ge, and B for charge compensation by the network modifier cations. Aluminum is found in a predominantly four-coordinated environment. Its anionic functionalization and, with second priority, that of the boron oxide component take precedence over that of the germanium oxide component. The glass transition temperature decreases with increasing B_2O_3 content and shows an excellent correlation with the average network connectivity deduced from the NMR data [55].

7. **References** (Certev faculty in yellow, international collaborators in green)

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Yellow = CeRTEV FACULTY. Green= INTERNATIONAL COLLABORATORS

EDUCATION AND OUTREACH

Ana CM Rodrigues (Coordinator) and Karina Lupetti (Researcher)

1. Development of professional qualification strategies in glass science and technology

The "Technician in Glass Production" course, a 3-semester course project conceived and realized in partnership with the Paula Souza Center, Abividro, and the glass company Nadir Figueiredo, has reached its maturity. Up to now, we have had already two cohorts of graduated students.

Of the 40 students enrolled in the course´s first cohort, 32 received their degree in July 2019. In the second cohort, which was concluded in December 2020, there were 27 graduations. To follow up on the professional progress of our graduates a questionnaire was sent to all the course participants. Out of the 16 responses received, 12 answered that they are working with glass production.

In 2021, there was a third selection via the Paula Souza Center, with 40 admitted students, from a pool of 65 applicants. Due to the Covid-19 crisis, face-to-face training was not possible. However, we had a remarkably interesting on-line training course devoted to hyalotechnics, the art of transforming glass or shaping it into labware products. 34 teachers participated, via Microsoft Teams, over a two-day period. For this activity, the hyalotechnician from the UFSCar chemistry department, gave various on-line demonstrations. Three videos were also recorded.

We also know that the Paula Souza Center is taking the necessary steps so that the course is recognized by the MEC (Ministry of Education and Culture) and thus can be offered throughout Brazil, not being limited to the São Paulo State.

Because of Covid-19, there has not been a new edition of the "CeRTEV Glass Technology Course" in the last twelve months. We are currently planning an online edition in August-September 2021

2. Diffusion of basic and glass science

From July 2020 to June 2021, we were all impacted by the social distancing imposed by Covid-19. Some of the traditional face-to-face activities were adapted to the online mode, while others were created to especially meet this demand.

Online workshops

During this period of pandemic, all face-to-face meetings were suspended, and the group adapted to the technology by holding weekly on-line meetings. Applications such as WhatsApp, Google Hangouts and Google Meet are being used to allow the continuity of the work carried out by the group. Workshops of 2 hours a week from April 2020 to June 2021 were carried out to discuss the theater play "QUI Remédio!" (What a medicine!). The creation and presentation of this play was postponed until the return of face-to-face activities is possible.

During this period the group also worked together on the adaptation of theatrical activities for the inclusion of people with visual impairment and reduced mobility in "Olhares Group". We also created and presented the theater videos "Cordel Periódico" (https://www.youtube.com/watch?v=tsbFaT8erbU); "What a medicine: vaccine!" (https://www.youtube.com/watch?v=FbKtQYnHmps), "Clepsidra: the case of water" (https://www.youtube.com/watch?v=CajJ7w1_MJ4&list=PLiDdRdfnvzg-DCvg593dnZQMbIw0pZ4fm&index=47) and " Chemistry by Table".

In-house scientist contest

4 hours of short course (October 24-31, 2020) by the Scientist at home, with two different times of 30 minutes each, with the participation of ~40 children/teenagers per day. 19 videos were recorded for the online minicourse.
https://www.youtube.com/watch?v=Dw3P8Zjykas&list=PLiDdRdfnvzg-8-2u32KzZ5aBd8_7o0czR
We had 80 entries, 28 finalist videos and 9 awarded videos in the categories 7 to 10 years old, 11 to 14 years old and 15 to 18 years old. The result may be seen at:
https://www.facebook.com/tvufscar/videos/1605806229606214

Theater workshops (September to December)

We performed the following theater workshops which resulted in videos uploaded on YouTube.

(i) "Jack and Halloween", the result of a children's theater creation workshop and performed by the groups Ouroboros and Olhares.
https://www.youtube.com/watch?v=Vi_j2CJuko4&list=PLiDdRdfnvzg-DCvg593dnZQMbIw0pZ4fm&index=45

(ii) " messages for Cantata 2020", the result of the adult theater workshop. Messages, songs and poems from Olhares Group and guests were recorded remotely and the two-hour event, consisting of 20 videos, was broadcast live on YouTube.
https://www.youtube.com/watch?v=uHrJTRV_wuk&list=PLiDdRdfnvzg9bEvNPNgEJmNPnfEIV-bSC
and
https://www.youtube.com/watch?v=tFCux0EtxzY&list=PLiDdRdfnvzg9bEvNPNgEJmNPnfEIV-bSC&index=15

Commemoration of 15 years of Ouroboros and 10 years of Olhares (virtual meetings)

15 meetings were held via Google Meet (15-29/10) with members and former members of the Ouroboros and Olhares Groups lasting 1.5 to 2.5 hours to record the history of these groups from the first theatrical productions to the current ones in 2020. The meetings were recorded and edited for online availability in celebration of the 15th anniversary.
https://www.youtube.com/watch?v=8ial43CzqDE&list=PLiDdRdfnvzg8LGQb4gAKnLJk9k4qmtU8J

XVII Circus of Science online in XVII National Science and Technology Week (NSTW) (October 17-23, 2020)

The website Circo da Ciência at FAI was developed and all the proposed activities are described (https://circodaciencia.faiufscar.com/#/)
Some meetings of the Ouroboros 15 years event were also held during the National Week of Science and Technology in 2020. 13 theater plays were edited and made available with audio description and exhibited on the Porão da Ciência channel. 28 videos of the group's photo-memories were also produced. Production of activities for

NSTW such as long and short theater plays, molecular cooking and scientific experiments videos are available on the link:
https://www.youtube.com/channel/UCFEkDzgivnK_Y8S8BZk_gmw/videos
The Circus of Science had the participation of other PET groups that in general developed videos and interactive online activities, but with a small synchronous participation of the general public. While interaction is certainly most effective in the face-to-face mode, the production of new contents and their on-line availability also serve to expand the dissemination of projects and should be incorporated into CeRTEV's future educational outreach efforts.
This online format can be improved, with more time for dissemination and personalized invitation to groups of students, thus, we believe that there will be greater synchronous interaction. Asynchronous activities were tracked until the end of the year to record the number of views and achievements of other possible scheduled interactions.
In the Porão da Ciência channel of the Ouroboros Center for Scientific Dissemination, we recorded 8490 views of the various videos available throughout the year.

VI Workshop on Scientific Dissemination and Playful Activities (12/13- 4 hours duration)
The COVID-19 pandemic also forced us to conduct the 2020 Workshop annually organized by Ouroboros (UFSCart) and CRECIN (ESALQ-USP) *on-line*. During the first part of the workshop nine abstracts of graduate and undergraduate were presented. In the second part, *on-line* interactive activities were carried out with forty-five participants, both with and without visual impairment.

Day of the Person with Disabilities (12/03/2020)
Documentary: Olhares
https://youtu.be/H7Kt_NQLVBw

Live Science on Stage
6 online lectures by Instituto Ciência em Cena with individual presentations by the science dissemination theater groups.

- 28/08/2020 FANATIcs of Chemistry (UERN- Mossoró) and Baobá (UFERSA-Mossoró)
- https://www.youtube.com/watch?v=3gaXC9sAMUo
- 25/09/2020 Ouroboros and Olhares (UFSCar- São Carlos)
- https://www.youtube.com/watch?v=J46moxAXA8Y
- 30/10/2020 Seara Science (UFC- Fortaleza) and Flogisto (UFPR- Ponta Grossa)
- https://www.youtube.com/watch?v=V4-LNunOwNw
- 11/27/2020 LetraFisic (UEMA- Caxias) and LicenciArte (UEMA- Caxias)
- https://www.youtube.com/watch?v=3nFWxMVkaak
- 02/04/2021 Alchemy (UNESP-Araraquara) and Chemistry in Action (USP-São Paulo) https://www.youtube.com/watch?v=4BEJeZzJXWw
- 05/07/2021 Test Tube (UECE- Itapipoca) and QuiTrupe (UNIFEI-Itajubá)
- https://www.youtube.com/watch?v=r_HTt5Xgh5s
- 06/25/2021Ciênica (UFRJ) and Lab Móvel (UFPR)
- https://www.youtube.com/watch?v=EoqlRmTtTMA

Live and *on-line* theater presentations

05-08 UFTM- Theater as a possibility for scientific dissemination
16/09 UFABC- Molecular gastronomy: the science and art of cooking
09/29 UTFPR- Molecular gastronomy: scientific aspects in the art of cooking
10/15 ATPC-DE of São Carlos. Ouroboros Center for Scientific Dissemination: science, art and inclusion.
10/29 UFSCar (Future Chemistry and Perspectives- Round table: dialoguing with graduates)
11/23 IQ/UFG- Molecular gastronomy: science and art
11/28- USP- Experiments on stage (There are girls in science)
02/11/2021 UFPR- Girls in Science (Workshop Scientist at home)
12/02/2021 Olhares and Ouroboros Groups (Unsubmissive project- Art and Science on Stage)
04/08/2021 (UERN- Mossoró) The Inclusive Art and Scientific Dissemination
and Poetry
10/08 Children's Day (CEMEI Marli Alves)- Science that laughs
11/21-22 Web House of Creation- Clepsydra: the case of water
04/08/2021- UERN-Mossoró - Chemical by table
06/14/2021 VI SMEQ- Periodical Cordel
06/17/2021 SIBICS São Carlos- Ouroboros: art, science and inclusion

Congress participation

- 05/24-27/2021 PCST 2020+1 Public Communication of Science and Technology (Virtual Conference)
- 05/13/2021 -Visual Presentation Museums, Exhibits and Art (Ouroboros: science, art and inclusion)
- https://conference.pcst.co/program/visuals
- 05/25/2021 Making PCST conferences as inclusive and diverse as possible (Project Olhares, Federal University of Sao Carlos)
- https://www.abdn.ac.uk/events/documents/PCST%202021%20Programmea.pdf

04/ 19-23/2021 IV JALEQUIM-IV National Meeting Of Games And Playful Activities In Teaching… (Virtual Conference)
04/19/2021 The science of vitreous materials illustrated in strips and the use of digital media as a means of dissemination (Iwata, A. Y.; Rodrigues, A. C. M; Lupetti, K.O.)
04/21/2021 Scientist at home: connected experiences (Maia, G.; Lupetti, K.O.)

The Vitreous Minute podcast series at Radio UFSCar completed more than 100 programs with the following new editions:

- **Programmed glasses** (Interviewee: Prof. Dr. Edgar Zanotto)
- https://www.radio.ufscar.br/podcast/minutovitreo-17-06-2020 /
- **Sustainable glass** (Interviewee: Prof. Dr. Hellmut Eckert)
- https://www.radio.ufscar.br/podcast/minutovitreo-24-06-2020 /
- **Is it just glass dust?** (Interviewee: Prof. Dr. Eduardo Bellini)
- https://www.radio.ufscar.br/podcast/minutovitreo-01-07-2020/
- **Glass X-rays?** (Interviewee: Prof. Dr. Valmor Mastelaro)
- https://www.radio.ufscar.br/podcast/minutovitreo-29-07-2020/

- **Spy cores within the matter?** (Interviewee: Prof. Dr. José Schneider)
- https://www.radio.ufscar.br/podcast/minutovitreo-05-08-2020/
- **Simulate a glass?** (Interviewee: Prof. Dr. José Pedro Rino)
- https://www.radio.ufscar.br/podcast/minutovitreo-12-08-2020/
- **Glass sensors made with laser?** (Interviewee: Prof. Dr. Marcelo Andreeta)
- https://www.radio.ufscar.br/podcast/minutovitreo-19-08-2020/
- **The black magic of glass** (Interviewee: Dr. Mauro Akerman)
- https://www.radio.ufscar.br/podcast/minutovitreo-26-08-2020/
- **Kalsman's paradox** (Interviewee: Eng. Ricardo Lanceloti)
- https://www.radio.ufscar.br/podcast/minutovitreo-02-09-2020/
- **Machine Learning and Glasses?** (Interviewee: Dr. Daniel Cassar)
- https://www.radio.ufscar.br/podcast/minutovitreo-09-09-2020/
- **Glass teeth?** (Interviewee: Dr. Lais Dantas)
- https://www.radio.ufscar.br/podcast/minutovitreo-16-09-2020/
- **Glass and optoelectronics** (Interviewee: Ms. Nilanjana Shasmall)
- https://www.radio.ufscar.br/podcast/minutovitreo-18-11-2020/
- **Have you ever heard of Nasicom?** (Interviewee: Dr. Adriana Nieto Munhoz and Dr. Jairo Felipe Ortiz)
- https://www.radio.ufscar.br/podcast/minutovitreo-25-11-2020/
- **Comic glass stories?** (Interviewee: Dr. Adriana Yumi Iwata)
- https://www.radio.ufscar.br/podcast/minutovitreo-02-12-2020/
- **Crystals in Glass: Science and Art** (Interviewee: Dr. Vladimir Fokin)
- https://www.radio.ufscar.br/podcast/minutovitreo-10-03-2021/
- **Glasses regenerating life?** (Interviewed: Prof. Dr. Murilo Crovace)
- https://www.radio.ufscar.br/podcast/minutovitreo-17-03-2021/
- **Trust theory or experiment?** (Interviewee: Helena Ramirez da Costa (doctoral student)
- https://www.radio.ufscar.br/podcast/minutovitreo-24-03-2021/
- **The alchemist of the glasses?**
- https://www.radio.ufscar.br/podcast/minutovitreo-31-03-2021/
- **Tube TVs turning into vitreous enamel?**
- https://www.radio.ufscar.br/escute/?s=minutovitreo-07-04-2021/
- **Influencing scientists?**
- https://www.radio.ufscar.br/escute/?s=minutovitreo-14-04-2021/
- **Glasses healing wounds?**
- https://www.radio.ufscar.br/escute/?s=minutovitreo-21-04-2021/
- **Enterprising Scientists?**
- https://www.radio.ufscar.br/escute/?s=minutovitreo-28-04-2021/
- **Plastic glass?**
- https://www.radio.ufscar.br/podcast/minutovitreo-05-05-2021/
- **Award-winning sulphide glass?**
- https://www.radio.ufscar.br/podcast/minutovitreo-12-05-2021/
- **Produce stronger glass with the periodic table?**
- https://www.radio.ufscar.br/podcast/minutovitreo-19-05-2021/
- **Glass smile?**
- https://www.radio.ufscar.br/podcast/minutovitreo-26-05-2021/
- **Cristal with laser?**
- https://www.radio.ufscar.br/podcast/minutovitreo-02-06-2021/

- **Devitrify the glass?**
- https://www.radio.ufscar.br/podcast/minutovitreo-09-06-2021/
- **What is common between glass, adrenaline and vaccines?**
- https://www.radio.ufscar.br/podcast/minutovitreo-16-06-2021/
- **Award-winning glass jellyfish?**
- https://www.radio.ufscar.br/podcast/minutovitreo-23-06-2021/
- **Is the future made of glass?**
- https://www.radio.ufscar.br/podcast/minutovitreo-30-06-2021/

Production of comic books and science comics

Researcher Adriana Yumi Iwata, supervised by Professor Karina Omuro Lupetti, developed her doctoral research in Scientific Dissemination and involved the production and analysis of the series: Histories of Glass in Comics. The thesis was defended in May 2020 at the Graduate Program in Chemistry at UFSCar. The comics can be read in Portuguese on the website: www.vidro.ufscar.br and in English:

- http://www.icglass.org/home/education/
- http://www.icglass.org/images/files/44-hq4_bioactive-glass_2nd-version-for-upload-compactado.pdf
- http://www.icglass.org/images/files/44-hq2_glass-recycling_2nd-version-for-upload-compactado-1.pdf
- http://www.icglass.org/images/files/44-hq3_optical-fiber_2nd-version-for-upload-compactado.pdf
- http://www.icglass.org/images/files/44-hq1_glass-world_2nd-version-for-upload-compactado-1.pdf

Ms. Iwata is currently a FAPESP JC-IV Scientific Journalism Scholar and is developing the Tirinhas de Vidro project with an analysis of the scope of this language for scientific dissemination on social networks.

- https://www.instagram.com/tirinhasdevidro/
- https://www.facebook.com/tirinhasdevidro
- https://twitter.com/tirinhasdevidro
- https://tirinhasdevidro.wordpress.com/

In addition to the 4 comics, an illustration of the play "The glass age" by the Ouroboros Center for Scientific Dissemination was made, completing the collection of 5 comics on glass.

- https://nucleoouroboros.wordpress.com/hqs-online/

Chemists in the kitchen (in home) 2020-2021

60 hours of curricular activities were developed for more than 80 undergraduate and graduate students from different universities and community people from different Brazilian States. During 3 months (nov-jan), themes related to science and cooking were discussed online among the participants of the course.

III Soirée Scientists Artists "in home" (06/18/2021)

This 2-hour activity took place on June 18, also in commemoration of the Chemist's Day. Due to the COVID-19 pandemic, the event celebrating the 50th anniversary of UFSCar's Chemistry Department was also held *online* through Google Meet and broadcast on

YouTube. The synchronous interaction between the participants who are scientists, chemists, students, professors, DQ technicians and guests took place amid statements by the first students Rosa Bonfá Rodrigues and Teresa Zambon and professor Annik Vivier from the Department of Chemistry, tributes to professors and members of community that left because of COVID and the pandemic and presentations of musical numbers, poetry recitations, exhibition of drawings and photographs. The event organized by the Ouroboros Center of Science Communication can be watched through the link:

- https://www.youtube.com/watch?v=LsEwqfglm6k

QUIPANC: Science, culture and gastronomy of wild plants (06/ 05, 12, 19 and 26/2021)
It was a 6-hour event for more than 100 undergraduate, graduate students from different universities and community people from different Brazilian States. Themes related to science, sustainability and cooking of wild plants were discussed online among the participants of the course.

CeRTEV new home page: www.certev.ufscar.br
It was developed during the last months by SIN-UFSCar specialists and will support all essential information about the project.

Eduscar:
Aside from promoting science divulgation with a focus on glass, CeRTEV also actively participates in the UFSCar`s overall mission of educational outreach to the general public.
Thus, the idea came to unite all existing educational efforts of FAPESP-funded CEPIDs and CNPq – funded INCTs (Institutos Nacionais de Ciencia e Tecnologia) based in the city of São Carlos with the mission of improving basic and fundamental public education in the municipality. The main message to get across was that São Carlos has two public and especially important universities (UFSCar and USP), with several internationally recognized research groups, and very qualified researchers. On the other hand, the fundamental and elementary public schools in the city suffer from the same problems as others across Brazil. Thus, how can these two universities contribute to raising the level of public-school education and the degree of success of their students? To answer this question, the EduScar project was created, an initiative of coordinators and professors who develop large projects in public universities in São Carlos, SP, together with the Coordinators of the Regional Teaching Directorate (State) and the Municipal Teaching Secretariat. EduSCar's mission is to actively interact with schools in the region in order to help improve the education system, disseminate science and technology and promote scientific education. Research centers linked to FAPESP and CNPq already promote numerous activities in science dissemination and popularization. The integration of all these activities tends to promote a synergistic effect that will benefit the education system of São Carlos in a more professional and forceful way.

EduSCar activities developed in the last 12 months:
1 – Organization of a pedagogical project and assistance in structuring a pedagogical project proposal (curriculum and materials in tune with the BNCC (Base Nacional Comum Curricular - Common National Curriculum Base). EMEB (Escola Municipal de Educação Básica - Municipal School of Basic Education) Ulysses Ferreira Picollo was

inaugurated in February 2020 and serves around 500 students in elementary school during their early years. Through this activity, we helped the aforementioned EMEB in structuring and executing the school's pedagogical process through face-to-face and virtual activities.

2. Orientation and application of didactic activities to 40 ICJ (Iniciação Científica Júnior – Junior Scientific Initiation) high school scholarship holders from Public Schools in the region of the city of São Carlos, SP.
Owing to the pandemic, various topics of science are being taught on the internet, including experimental activities with the Arduino computational environment, taught by Professor Dr. Wilma Barrionuevo. During Arduino classes, students received theoretical instructions and educational kits so that they could do practical activities in their homes. The various experiments involved home automation, vegetable gardens, car parks, remote feeding of PETs, presence detectors, audible alarms, among others.
Prof. Sergio Motta and Profa Rosane gave classes on environmental issues and youth protagonism.
Topics related to chemistry, gastronomy, and materials such as glass were also addressed with the director of the Ouroboros Center for Scientific Dissemination, Dr. Karina Omuro Lupetti, in 5 weeks of interaction with lectures and demonstrations of experiments in chemistry, cooking and scientific aspects and the play Clepsidra: the case of water, performed by the group Olhares. Instigating curiosity and introducing students to the scientific method were the main objectives of these classes, which were administered by retired professor Dr. Rosa Bonfá Rodrigues, and by UFSCar students Giovanna Maia and Camila Rodrigues to share their experiences in gastronomy, chemistry, and biology, respectively. Dr. Marcelo Adorna Fernandes from UFSCar and Daniel da Costa e Silva Coelho, criminal officer expert in the State of Mato Grosso were invited to talk about Astronomy and Forensic Chemistry, respectively.
The next step is the development of the students' scientific projects that will be guided by the teachers and presented at a workshop in the second half of 2021.

3 - Launch of the Science from Home Challenge for public schools in 7 municipalities. Science challenges were launched, with different themes, following the curricula of either Elementary Schools (final years) or High Schools. Students produced videos and posted them on Facebook and on the Education Board page. In this context, 20 USP (University of São Paulo) residents in the areas of physics, mathematics, and science assisted in the elaboration and evaluation of activities sent to students from the State School of Integral Teaching Profa. Maria Ramos.

EduSCar Coordinators:
Prof. Dr. Edgar Zanotto – CEPID-CeRTEV, DEMa, UFSCar
Prof. Dr. Elson Longo – CEPID Department of Chemistry - UFSCar
Prof. Dr. Vanderlei Salvador Bagnato CEPID-CEPOF / IFSC / USP
Prof. Dr. Glaucius Oliva - CEPID IFSC, USP
Prof. Dr. José Alberto Cuminato ICMC CEPID / CEMEAI / USP
Profa. Dr. Deisy das Graças de Souza - PPGPsi-UFSCar
Profa. Dra. Arlene Gonçalves Correa - DQ-UFSCar / CERSUSCHEM
Profa. Debora G. C. Blanco - Director of the State Board of Education
Prof. Orlando Menegati - Municipal Secretary of Education

Profa. Dra. Wilma R. Barrionuevo: Executive Coordinator of EduSCar

International Year of Glass – 2022 – planned activities
The United Nations (UN) General Council on its meeting held on Tuesday 18th May 2021 have approved the application from The International Commission on Glass (ICG), along with the Community of Glass Associations (CGA) and International Committee for Museums and Collections of Glass (ICOM-Glass), to promote an International Year of Glass in the year of 2022.
The IYOG is a great opportunity to show society, in general, the importance of understanding and researching the glass material, its versatility, and all the innovative applications currently under development.
Thus, CeRTEV is planning some activities to celebrate IYOG and spread glass's importance in our lives.

- English translation of the comics in Mangá style, HQ "Tirinhas de Vidros"
- To illustrate a calendar with these comics, underlying important events in glass history.
- To make videos with the idea to disseminate the importance of glass in our modern society.
- To organize a special "symposium on glass",

To organize and inaugurate the "Museum of Glass", at UFSCar Campus, near LaMaV.

INNOVATION AND TECH TRANSFER
Eduardo Bellini Ferreira – EESC/USP (Coordinator)
Edgar Dutra Zanotto – DEMa/UFSCar
Oscar Peitl – DEMa/UFSCar
Sergio Luis da Silva – UFSCar (Tech Transfer Manager)

In the period between Jun/2020 and Jul/2021, we have pursued new technologies in all the fields of the main CeRTEV's plan and their transfer to the productive sector, following the same approach of last years based on the three pillars: i) establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry, focusing the skills of our group to bring the industry close to our academic institutions, connecting universities, companies, and other institutions through cooperation programs as PITE and PPP/FAPESP, and FINEP; ii) nucleation of spin-off companies from the group activities, stimulating entrepreneurship, and encouraging engagement in applications, such as PIPE/FAPESP; and iii) promotion of innovation and technology transfer, accomplished by our extensive know-how in these subject areas combined with the assistance of agencies at UFSCar (www.inovacao.ufscar.br) and USP (www.inovacao.usp.br). Below, we report our Innovation and Tech-transfer effort to channel CeRTEV's research achievements into innovation.

1. Establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry in this period
E.D. Zanotto has been working on joint projects with the following companies: **AGC (Japan)** (11/2019-10/2020): novel glass-ceramics (**76,200 €**) and (11/2020-10/2021) (**+76,200 €**); **IVOCLAR AG (Liechtenstein)** (11/2019-10/2020) (**54,000 €**): dental materials and (11/2020-02/2022) (**+27,000 €**); **CBMM (Brazil)** (Jan-December 2021):

optical and lead-free "crystal" glasses (**R$ 230.000, or 38,000 €**).
E.D. Zanotto chaired up to April/2019 the Scientific Council of the INSTITUTO SERRAPILHEIRA, the first private research foundation within Brazil. He is currently a member of the Board of Directors.
H. Eckert has ongoing projects with the **Nippon Electric Glass (Japan)** (01/2019-03/2021) on the structure-property relations for crack-resistant glasses (**40,000 €**); and **Schott Glass Company (Germany)** (04/2020-04/2022) on structural characterization of fluorophosphate glasses (**30,000 €**). A new contract with **Nippon Electric Glass (Japan)** is currently in the review process through the USP committees and is expected to start after 07/2021 (**40,000 €**).
M.R.B. Andreeta had a project with the company **Alacer Biomédica (Brazil) (**01/2018-06/2021) on the *Development of solid-state pH sensors*, a systematic study on the preparation of new vitreous and glass-ceramic systems based on borosilicates as solid-state pH sensors (**R$ 244,340.40**).
A.C.M. Rodrigues has an ongoing project with the **International Commission on Glass** (ICG) (**2.000 €**). Due to the Pandemic, the money has not been spent yet; and a project under negotiation with **CEBRACE (Brazil)**: "Recovery of glass polishing residue", to be submitted to Embrapii-UFSCar; the company has accepted the budget, and we are discussing aspects of intellectual property (**Embrapii+UFSCar+CEBRACE ~ R$ 600,000.00**)
E.B. Ferreira has a project under negotiation with the joint companies **BRAMAGRAN, CAJUGRAM and MAGBAN (Brazil)**: "*Artificial rocks obtained from mineral waste*"; the company has accepted the budget, and we are in the final stage of contract elaboration (**~R$ 600,000.00**).
M. Nalin has been negotiating two projects with Brazilian companies on glass, mediated by ABIVIDRO, i) incorporation of glass into asphalt mix and ii) new materials to prevent bird collisions on glass. Unfortunately, these projects were not continued, partially due to cost cuts attributed to the COVID Pandemic.
Further actions for establishing cooperation agreements will be considered according to the research advances made in each area.

2. Nucleation of spin-off companies from the group activities

VETRA Biomaterials, a CeRTEV spin-off company, founded in São Carlos in August 2014, offers glass and GC biomaterials combining unique biodegradability, bioactivity and bactericidal action. The company has actively participated in outreach activities promoted by CeRTEV and collaborated in pre-clinical and clinical research with several departments from various universities (Unicamp, Unifesp, Unesp, USP, UFABC). The VETRA-CeRTEV partnership has produced active and high-impact research and published eight scientific papers between June/20 and June/21. Nowadays, the company is incubated at Supera Parque (Ribeirão Preto-SP) and has already established its lean production plant. Two FAPESP projects (PIPE 2019/09099-6 and 2020/09584-9) and a FINEP challenge (*Mulheres Inovadoras*) are currently running. The company also has a FAPESP project in collaboration with the Department of Medicine at USP. VETRA has recently obtained a private investment from Jacto, an important Brazilian group, supplying contracts with two other national companies and is developing new technologies for dentistry and medical use.

3. Promotion of innovation and technology transfer

3.1. Patent applications

As results of our scientific & technological efforts, the following patent applications have been filed with the Brazilian National Institute of Industrial Property (INPI):

- BR 10 2020 023996-1, C.V. Rosa Machado, **E.D. Zanotto**, M.C. Crovace & **O. Peitl**, UFSCar, DEMa, 25/11/2020, "BIOACTIVE GLASS-CERAMIC BASED CEMENT (BIOSILICATE) FOR APPLICATIONS IN ORTHOPEDICS AND DENTISTRY," (in Portuguese).
- BR 10 2020 017697-8, **E.D. Zanotto**, C. Abadia, C. Chinaglia, M.T. Souza & M.C. Crovace, UFSCar, DEMa, 31/08/2020, "METHOD OF PREPARING SCAFFOLDS OF BIOSILICATE/BIOGLASS F18 AND SCAFFOLDS OBTAINED FOR APPLICATIONS IN MEDICINE AND DENTISTRY," (in Portuguese).
- BR 10 2021 007715-8, **E.D. Zanotto**, G.L. Santana, A.J.A. de Oliveira & M. Crovace, UFSCar, DEMa, 22/04/2021, “MAGNETIC COMPOSITE IN BIOACTIVE VITREOUS MATRIX FOR BONE TUMOR HYPERTHERMIA,” (in Portuguese).

The analysis at INPI, unfortunately, may take from 7 to 10 years.

3.2. Other actions for the promotion of innovation and technology transfer

3.2.1 Developing of equipment & scientific instrumentation devices carried out by the CeRTEV researchers:

- **Development of a viscosimeter for high viscosities**: currently, commercial high-temperature viscosimeters (600 to 1600 °C) are designed for the range of 10 to 10^{11} Pa.s, but none of them covers this range entirely, and three devices based on different techniques are needed, for example, the torque rotational cylinder (10 to $10^{3.5}$ Pa.s), parallel plates (10^4 to 10^8 Pa.s), and fiber stretching (10^8 to $10^{11.5}$ Pa.s). At relatively low temperatures and the highest viscosity for practical determination, the glass transition temperature (T_g) is usually determined by calorimetry (e.g., DSC) and related to its average characteristic viscosity (10^{12} Pa.s). However, there is no commercial viscosimeter operating above T_g. **O. Peitl** in LaMaV/DEMa-UFSCar designed a new beam-bending viscometer (Figure I) for up to $10^{16.5}$ Pa.s, although the literature reports this technique is applied for 10^8 to 10^{13} Pa.s. The new ***EDOS-HiV*** viscosimeter will be used for determining the glass structure relaxation phenomena in the viscosity range beyond 10^{13} Pa.s, which is crucial for a worldwide impacting check of the Classical Nucleation Theory.

Figure I. Building steps of the new ***EDOS-HiV*** viscosimeter.

- **Three-balls-on-ball device** is intended to measure disc samples mechanical strength rather than 3- or 4-point bending tests, which need hard conditioning work for specimen edges. **O. Peitl** built two ball-on-three-ball sample holders, which can be seen in Figure II.

Figure II. Three-balls-on-ball devices.

○ **Pre-cracking device**: **O. Peitl** designed and built an instrument (Figure III) for the stable propagation of cracks previously produced by an indentation in microhardness equipment. The controlled crack propagation is essential for determining fracture toughness (K_{IC}) of fragile materials like glass and glass-ceramics to develop tougher microstructures.

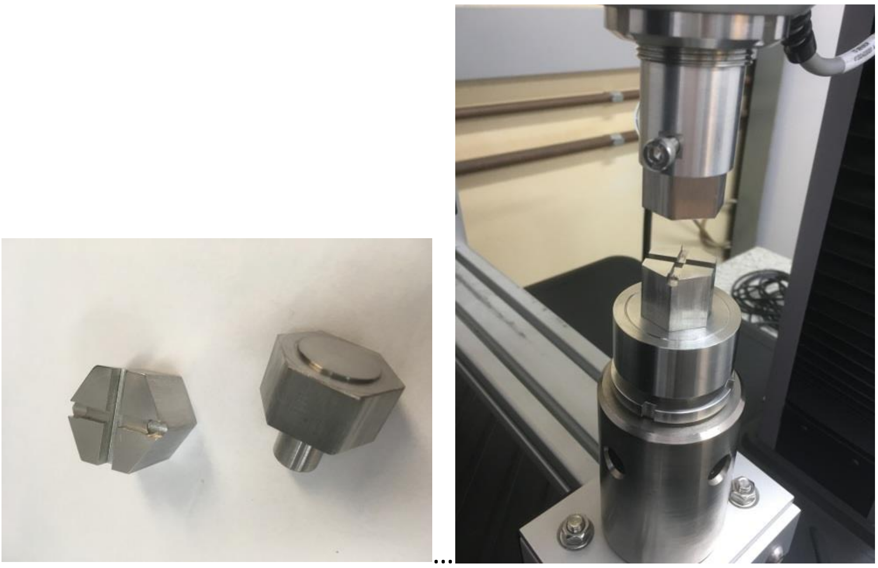

Figure III. Pre-cracking device for K_{IC} determination.

○ **Ion-exchange sample holder**: the ion exchange process in glass-ceramics is carried out with a device developed by O. Peitl at LaMaV/DEMa-UFSCar, consisting of three individual pieces: 100 x 70 x 60 mm bath box in 316 stainless steel, hollow 316 stainless steel support for the samples (Figure IV), and a hook for removal from the oven box. The salt used for the bath is deposited inside the container, placed in a muffle oven heated to the desired temperature, and maintained until all the salt is in its liquid phase. Then, disc-shaped specimens of approximately 1.2-mm thickness are supported on the hollow support so that both surfaces can be treated without any contact.

Figure IV. Ion-exchange sample holder.

- **Casting molds for sample production**: several molds were produced by **O. Peitl** from different materials suitable for the type of glass and aim of the analysis. Among the materials, we highlight graphite, copper brass, and stainless steel (Figure V).

Figure V. Graphite, copper brass, and stainless steel molds.

- **Flash-sintering system**: during the M.Sc. course supervised by **E.B. Ferreira** (EESC-USP) and **C. Magon** (IFSC-USP), J.M. Murdiga took an artificial intelligence course and applied the knowledge acquired on image analysis, allowing much more precise and complete monitoring of the phenomenon. With a reliable furnace system mentioned in the previous report, the flash-sintering team updated the software used in the Flash Sintering apparatus. The new software can now automatically detect the specimen length through its geometry, using circle detection algorithms (Figure VI). With the correct image treatment, measuring the specimen size every 16.6 milliseconds allows the process to be analyzed quickly and accurately.

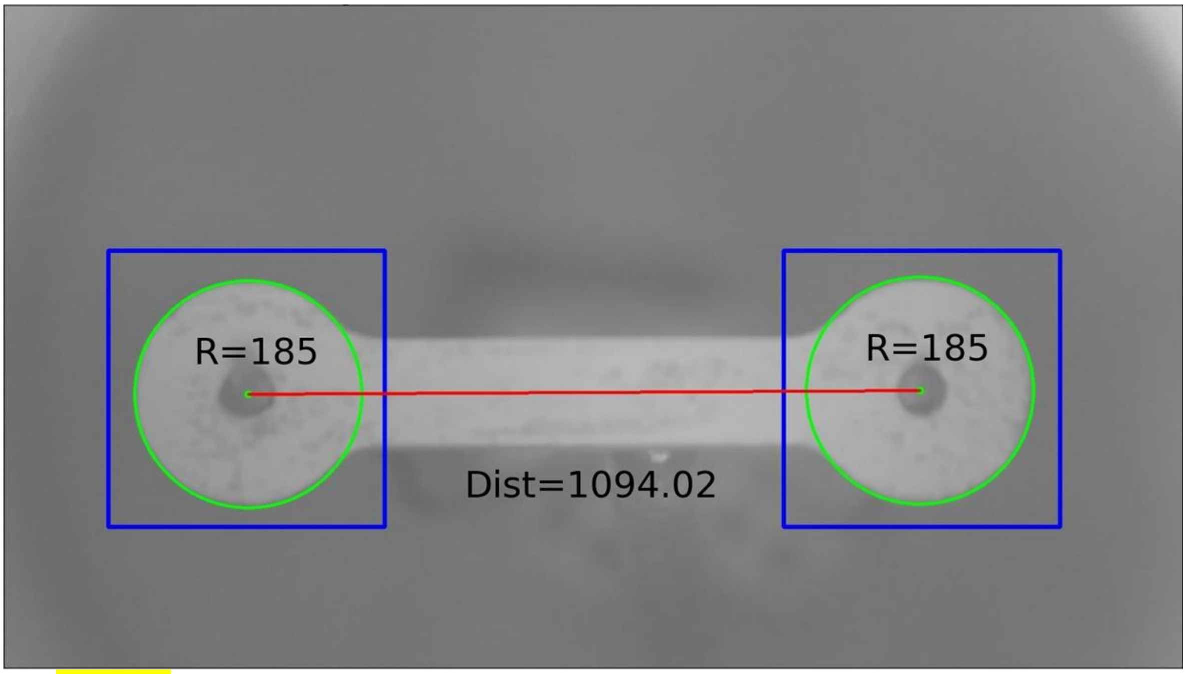

Figure VI. New software for automatic sample length detection allows the flash sintering apparatus to perform optical dilatometry with an electrical field applied.

○ Although Covid-19 slowed down our experimental research efforts last year, we have implemented a new installation in the CeRTEV infrastructure for glass laser melting (Figure VII). This technique is based on an aerodynamic levitation system using compressed air. Using this technique, the M. Sc. student Maíra Dombroski Neme, supervised by **M. Andreeta** (DEMa-UFSCar), successfully developed a new methodology to produce miniaturized solid-state pH sensors (patent pending). We were able to identify changes in standard pH solutions in the range of pH= 2 to 10. With acquiring a new electrometer, we will explore the developed methodology to improve/optimize the sensor.

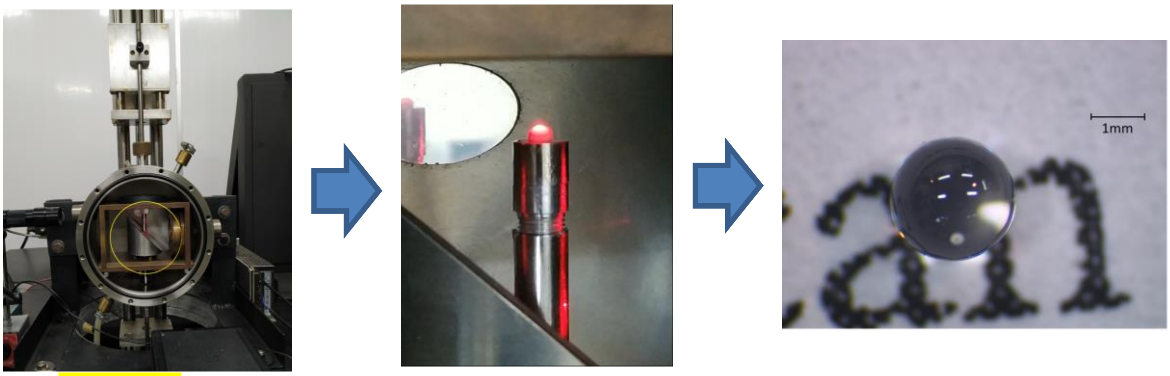

Figure VII. New installation in the CeRTEV infrastructure for glass laser melting.

○ EPR spectrometers offer a non-destructive analytical technique for detecting paramagnetic species for local atomic structure analysis. Our group has an EPR laboratory at IFSC-USP equipped with a commercial Continuous-Wave (CW) and pulsed EPR spectrometer to exploit the nature of paramagnetic centers in glasses. **C. Magon** built a second **CW-EPR spectrometer** based on a few Bruker parts discarded by other Brazilian laboratories. The built spectrometer is shown in Figure VIII. The components: microwave bridge, magnet and magnet power supply are original from Bruker but restored by our group. We developed all the control and data acquisition electronics and the computer software program based on LabVIEW. The field controller unit is still original from Bruker (also restored by us), but it will be replaced by our new controller that is under development. Shortly, we also plan to build a self-made microwave bridge for CW-EPR. Tests are in progress to evaluate the performance of the new spectrometer.

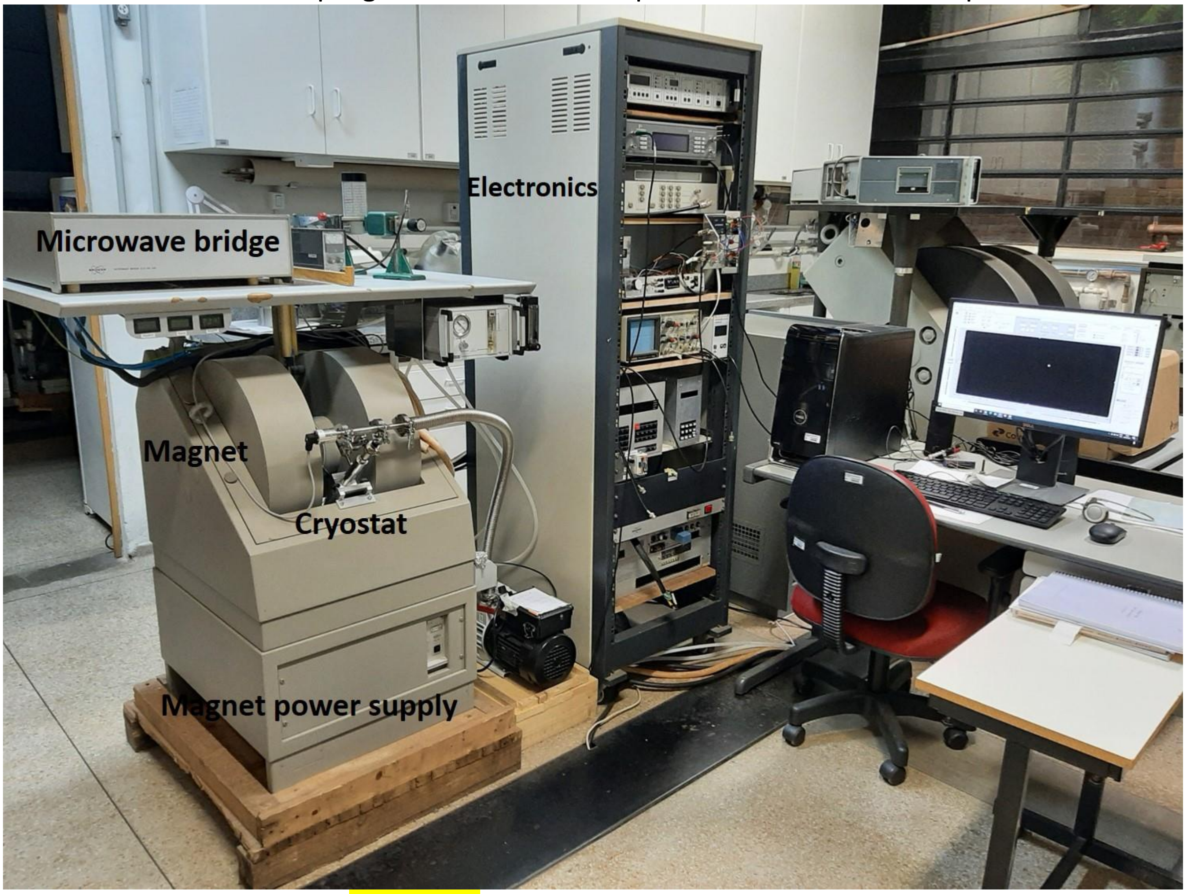

Figure VIII. CW-EPR spectrometer.

3.2.2. Other actions for promoting innovation and technology transfer

- I.N. Piccirillo kept developing a platform for collaborative technology development with the industry in the CeRTEV environment aiming to facilitate the product and technology development process and manage Intellectual Property based on roadmapping and blockchain technology. Prof. D.C. Amaral supervises her Ph.D. thesis at the Industrial Engineering Department at USP-São Carlos. The goals are to increase the agility of the technological cooperation process by minimizing risks regarding the exposure of sensitive data, reducing transaction costs for licensors and licencees, making this process more efficient. This project spun off into a startup called Lotik, selected among the 10 in Brazil for the Swissnex Academy-Industry Training (Swissnex AIT) program to help researchers-entrepreneurs from Switzerland and Brazil develop their projects for the market and industry. The Training Camp is held in both countries and provides an immersion in innovation and entrepreneurship environments. The project was also selected for the CATALISA ICT (SEBRAE), a journey to accelerate and encourage researchers, from academia to the market, including selection gates based on merit criteria regarding the proposal's potential for innovation.
- **A.C.M. Rodrigues** organized the CeRTEV Course on Glass Technology for glass professionals, with Glass Industry and University lecturers. Unfortunately, this training

course was also canceled due to the Pandemic. The "CeRTEV Glass Technology Course 2020" was planned in São Carlos, from March 30 to April 4, 2020, with participants from different glass industries in the whole country. Because of the impossibility of taking face-to-face classes, we plan an online course for August/September 2021, together with the Glass Commission of the Brazilian Ceramic Society (ABCeram).

○ We held the *III Workshop University-Industry (WUI) in Vitreous Materials*, virtually, in November/2020, with the scope of presenting a Technology Roadmap for the Glass Industry in Brazil. Preparing workshops (33 h over three months) were developed with the Glass Commission of the Brazilian Ceramic Society, most of which are in the National Advising Board of CeRTEV. A team of eleven was formed with three multinational companies, six senior consultants, two principal researchers (**E.B. Ferreira** & **A.C.M. Rodrigues**), and I.N. Piccirillo as the roadmapping specialist. A summary roadmap and five thematic roadmaps (TRM) were created based on current main technical challenges in glassmaking: glass forming, glass homogeneity, raw materials, defects in glasses, and foam during glass melting, selected during the stage of scope searching and challenge detection in the glass sector. For the final presentation, the participants were invited directly by email and indirectly by sharing the website link on social networks (Linkedin and Whatsapp) and published on Brazil's largest leading online event platform (Sympla). We had 220 attendees from 42 companies and 19 universities and technical schools, a fantastic threefold increase compared to the first two WUI Vitreous Materials conducted in person. A virtual platform was developed by Kosmos Brasil, allowing for an immersive and interactive environment. The roadmapping methodology, each sectorial roadmap and the final TRM were presented in 30 min with another 15 min for interaction with the public. An online questionnaire was sent to the participants during presentations to list collaboration interests and suggest technological solutions and improvements. The final RoadMap is shown in Fig. IX, constituting an essential guide for glass development in Brazil.

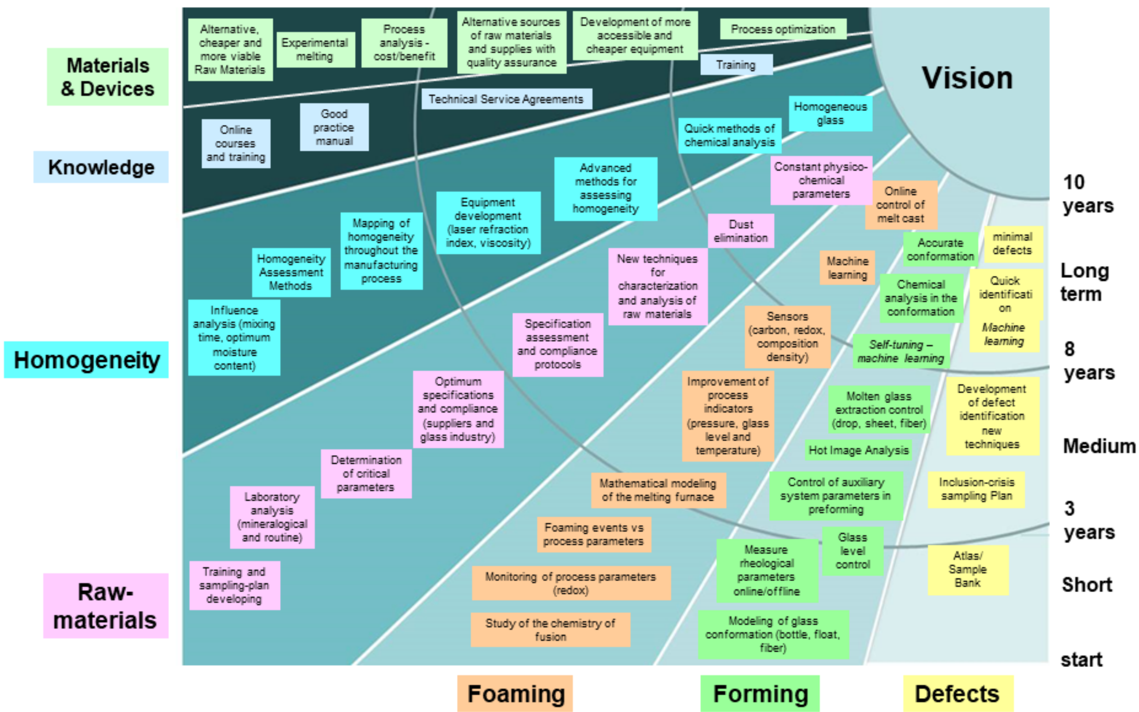

Figure IX. Technology Roadmap for the Glass Industry in Brazil.

○ **E.B. Ferreira** and part of the TRM team lectured in the course Glass: Nature, Structure and Properties, in the Virtual Glass School on June 07-30, 2021, organized by the Glass Commission of the Brazilian Ceramic Society, as one demand for training detected during the TRM effort, for professionals in the glass sector.

○ In the **COVID-19 Pandemic**, the use of digital tools is a prerequisite for partners to interact remotely. In one case study, entitled *University-industry involvement through digital events and roadmap in COVID-19 pandemic crisis*, authored by I. Piccirillo, D.C. Amaral, M.G. Oliveira & E.B. Ferreira, and to be presented in the R&D Management Conference 2021, July 6-7, 2021, we learned about the virtual involvement between the university and industry with the support of roadmapping. There was an improvement in communication between the participants, which was unexpected, as the most accepted hypothesis has been that face-to-face activities lead to the highest interaction benefit. Therefore, this case study indicates that roadmapping is an alternative instrument for UIC preparation through virtual involvement. The virtual participation enabling tools were a) Miro, an online collaborative platform for interaction and layout development, b) Google Meet to allow verbal communication and screen sharing, and c) Google Drive for document sharing. The digital collaboration by itself did not influence the involvement of universities and engagement for cooperation. However, the presentation based on roadmapping on different themes increased the interest in a partnership. Some advantages of using roadmapping have been confirmed in the university-industry collaboration. According to the organizers, the core team (11 participants) only attended the whole roadmapping process due to the possibility of remote participation. If it were conducted as physical meetings, it would have been impossible to deliver the same involvement due to time and financial constraints. Roadmapping also supported the preparation for collaboration. It encouraged the simultaneous participation of competitive and non-competitive universities and industries. This involvement was essential for roadmapping updates concerning priorities and a greater understanding of the glass industry challenges. In addition, ABCeram was a crucial stakeholder in generating partnerships between competitive, non-competitive, and university partners. It can give a neutral environment to solve possible tensions between cooperation and competition faced by resistance and conflicts. The split into five sectorial roadmaps due to the complexity of the glass industry facilitated the search for dedicated technical solutions to problems of the most significant interest of the participants. Experience showed that it was a valid strategy. The presented solution was a quick response to the current COVID-19 crisis. This experience showed that virtual involvement in collaboration can reach beyond harm reduction. With the use of the roadmapping technique, it is possible to obtain virtual results even better than face-to-face. Considering that roadmapping could not be developed at the same level of participation in a face-to-face effort, the virtual model presents clear advantages and new opportunities.

3.2.3. Publication of glass-technology related articles

Optical glass-ceramics

▪ CASSAR, D.R., SANTOS, G.G., **ZANOTTO, E.D.** Designing optical glasses by machine learning coupled with a genetic algorithm. *Ceramics International* 47 [8] (2021) 10555-10564.

- FERREIRA, P.H.D., FABRIS, D.C.N., VILLAS BOAS, M.O.C., BEZERRA, I.G., MENDONÇA, C.R., **ZANOTTO, E.D.** Transparent glass-ceramic waveguides made by femtosecond laser writing. *Optics and Laser Technology* 136 (2021) 106742.
- SOARES, V.O., SERBENA, F.C., OLIVEIRA, G.D.S., DA CRUZ, C., MUNIZ, R.F., **ZANOTTO, E.D.** Highly translucent nanostructured glass-ceramic. *Ceramics International* 47 [4] (2021) 4707-4714.
- PAN, L., DAGUANO, J.K.M.F., TRINDADE, N.M., CERRUTI, M., **ZANOTTO, E.D.**, JACOBSOHN, L.G. Scintillation, luminescence and optical properties of Ce-doped borosilicate glasses. *Optical Materials* 104 (2020) 109847.

Bio and dental glasses and glass-ceramics

- QUEIROZ, M.B., TORRES, F.F.E., RODRIGUES, E.M., VIOLA, K.S., BOSSO-MARTELO, R., CHAVEZ-ANDRADE, G.M., SOUZA, M.T., **ZANOTTO, E.D.**, GUERREIRO-TANOMARU, J.M., TANOMARU-FILHO, M. Development and evaluation of reparative tricalcium silicate-ZrO2-Biosilicate composites. *Journal of Biomedical Materials Research - Part B Applied Biomaterials* 109 [4] (2021) 468-476.
- ELSAYED, H., COLOMBO, P., CROVACE, M.C., **ZANOTTO, E.D.**, BERNARDO, E. Suitability of Biosilicate® glass-ceramic powder for additive manufacturing of highly porous scaffolds. Ceramics International 47 [6] (2021) 8200-8207.
- BERNARDO, E., ELSAYED, H., ROMERO, A.R., CROVACE, M.C., **ZANOTTO, E.D.**, Fey, T. Biosilicate® Glass-Ceramic Foams From Refined Alkali Activation and Gel Casting. Frontiers in Materials 7 (2021) 588789.
- SOARES, V.O., SERBENA, F.C., MATHIAS, I., CROVACE, M.C., **ZANOTTO, E.D.** New, tough and strong lithium metasilicate dental glass-ceramic. *Ceramics International* 47 [2] (2021) 2793-2801.
- PASSOS, T.F., SOUZA, M.T., **ZANOTTO, E.D.**, DE SOUZA, C.W.O. Bactericidal activity and biofilm inhibition of F18 bioactive glass against Staphylococcus aureus. *Materials Science and Engineering C* 118 (2021) 111475.
- SILVA, L.D., PUOSSO, F.C., SOARES, V.O., **PEITL FILHO, O.**, SABINO, S.D.R.F., SERBENA, F.C., CROVACE, M.C., **ZANOTTO, E.D.** Two-step sinter-crystallization of K2O–CaO–P2O5–SiO2 (45S5-K) bioactive glass. *Ceramics International* (2021).
- OLIVEIRA, V.C., SOUZA, M.T., **ZANOTTO, E.D.**, WATANABE, E., CORAÇA-HUBER, D. Biofilm formation and expression of virulence genes of microorganisms grown in contact with a new bioactive glass. Pathogens 9 [11] (2020) 0927, 1-15.
- DE ARAÚJO LOPES, J.M., BENETTI, F., REZENDE, G.C., SOUZA, M.T., CONTI, L.C., ERVOLINO, E., JACINTO, R.C., **ZANOTTO, E.D.**, CINTRA, L.T.A. Biocompatibility, induction of mineralization and antimicrobial activity of experimental intracanal pastes based on glass and glass-ceramic materials. *International Endodontic Journal*, 53 [11] (2020) 1494-1505.
- BRANDÃO, S.M., SCHELLINI, R.A., **PEITL, O.**, **ZANOTTO, E.D.**, MATAYOSHI, S., MENEGHIM, R.L.F.S., SCHELLINI, S.A. Conical Biosilicate Implant for Volume Augmentation in Anophthalmic Sockets. *The Journal of Craniofacial Surgery* 31 [6] (2020) 1838-1840.
- BENETTI, F., BUENO, C.R.E., DOS REIS-PRADO, A.H., SOUZA, M.T., GOTO, J., DE CAMARGO, J.M.P., DUARTE, M.A.H., DEZAN-JÚNIOR, E., **ZANOTTO, E.D.**, CINTRA, L.T.A. Biocompatibility, biomineralization, and maturation of collagen by rtr®, bioglass and dm bone® materials. *Brazilian Dental Journal* 31 [5] (2020) 477-484.

- CRUZ, M.A., FERNANDES, K.R., PARISI, J.R., VALE, G.C.A., JUNIOR, S.R.A., FREITAS, F.R., SALES, A.F.S., FORTULAN, C.A., **PEITL, O.**, **ZANOTTO, E.D.**, GRANITO, R.N., RIBEIRO, A.M., RENNO, A.C.M. Marine collagen scaffolds and photobiomodulation on bone healing process in a model of calvaria defects. *Journal of Bone and Mineral Metabolism* 38 (5) (2020) 639-647.
- PARISI, J.R., FERNANDES, K.R., APARECIDA DO VALE, G.C., DE FRANÇA SANTANA, A., DE ALMEIDA CRUZ, M., FORTULAN, C.A., **ZANOTTO, E.D.**, **PEITL, O.**, GRANITO, R.N., RENNÓ, A.C.M. Marine spongin incorporation into Biosilicate® for tissue engineering applications: An in vivo study. *Journal of Biomaterials Applications* 35 [2] (2020) 205-214.
- MONTAZERIAN, M., **ZANOTTO, E.D.**, MAURO, J.C. Model-driven design of bioactive glasses: from molecular dynamics through machine learning. *International Materials Reviews* 65 [5] (2020) 297-321.
- UBALDINI, A.L.M., PASCOTTO, R.C., SATO, F., SOARES, V.O., **ZANOTTO, E.D.**, BAESSO, M.L. Effects of bioactive agents on dentin mineralization kinetics after dentin bleaching. *Operative Dentistry* 45 [3] (2020) 286-296.
- MARQUES, D.M., OLIVEIRA, V.D.C., SOUZA, M.T., **ZANOTTO, E.D.**, ISSA, J.P.M., WATANABE, E. Biomaterials for orthopedics: anti-biofilm activity of a new bioactive glass coating on titanium implants. *Biofouling* 36 [2] (2020) 234-244.
- MARIN, C.P., SANTANA, G.L., ROBINSON, M., WILLERTH, S.M., CROVACE, M.C., **ZANOTTO, E.D.** Effect of bioactive Biosilicate®/F18 glass scaffolds on osteogenic differentiation of human adipose stem cells. *Journal of Biomedical Materials Research - Part A*, (2020).
- CARMINATTI, M., BENETTI, F., SIQUEIRA, R.L., **ZANOTTO, E.D.**, BRISO, A.L.F., CHAVES-NETO, A.H., CINTRA, L.T.A. Experimental gel containing bioactive glass-ceramic to minimize the pulp damage caused by dental bleaching in rats. *Journal of Applied Oral Science* 28 (2020) e20190384, 1-10.

Miscelaneous

- MONTAZERIAN, M., **ZANOTTO, E.D.** Tough, strong, hard, and chemically durable enstatite-zirconia glass-ceramic. *Journal of the American Ceramic Society* 103 [9] (2020) 5036-5049.

- ALCOBAÇA, E., MASTELINI, S.M., BOTARI, T., PIMENTEL, B.A., CASSAR, D.R., DE CARVALHO, A.C.P.D.L.F., **ZANOTTO, E.D.** Explainable Machine Learning Algorithms For Predicting Glass Transition Temperatures. *Acta Materialia* 188 (2020) 92-100.
- BORGES, A.L., SOARES, S.M., FREITAS, T.O.G., OLIVEIRA JÚNIOR, A., **FERREIRA, E.B.**, FERREIRA, F.G.S. Evaluation of the Pozzolanic Activity of Glass Powder in Three Maximum Grain Sizes. *Materials Research* 24 [4] (2021) e20200496.

4. Plan for the next period

Besides the general plan of pursuing new technologies in all the fields of our CeRTEV project and their transfer to the productive sector, based on our strategy given at the beginning of this report, we will also invest effort in the following goals:

- The ***4th Workshop University-Industry on Glass Materials*** will be held, if possible at EESC-USP in São Carlos, aiming to identify demands on glass science and technology from the national glass industry. The event is organized in cooperation with our National Advisory Board, most of whose members also make the Commission on Glass of the

Brazilian Ceramic Society. The focal theme of this workshop will probably be the International Year of Glass 2022.

- We will continue our efforts to boost the **Wikividros**, the Web-based content on glass science & technology, created by CeRTEV as an open collaboration platform hosted at https://wikividros.eesc.usp.br/.
- Even though economic and political issues prevented us from making significant progress on this matter, we maintain our plan of launching a program of internship training and vacation school of undergrad and graduate students from CeRTEV with partners from the glass industry, following the suggestion of H. Jain, member of CeRTEV's IAB.

Funding from industry 2020 – 2021

EDGAR DUTRA ZANOTTO
ACG (Japan) - Euros 152,400 - Nov. 2019 - Oct. 2021
IVOCLAR AG (Liechtenstein) - Euros 81,000 - Nov. 2019 - Feb. 2022
CBMM (Brazil) - R$ 230.000 - Jan. - Dec. 2021

HELLMUT ECKERT
Nippon Electric Glass - Euros 40,000 Jan. 2019- Mar.2021
Schott Glass AG - Euros 30,000 April 2020- March 2022

MARCELLO RUBENS BARSI ANDREETA
Alacer Biomédica - R$244.340,40 - Jan. 2018 - Jun. 2021

Funding from other agencies: CNPq, CAPES, International agencies

H. ECKERT, CNPq, Universal - R$ 37,500 2020-2022
H. ECKERT, DFG, SFB858 €78,375, 2020-2021
H. ECKERT, DFG, Ec168-20 € 10,000, 2019-2021
E.D. ZANOTTO, CNPq, Universal - R$ 40.000 2019-2021
A. S. S. DE CAMARGO, FAPESP, Auxílio Regular - R$ 113.000,00, 2020 a 2022
J.F. SCHNEIDER, FAPESP, Programas Especiais / EMU - Equipamentos Multiusuários, US$ 248.250,00, 2019-2026
V. R. MASTELARO, CNPq, Universal, R$ 45.000.00 - 2020-2022
M. NALIN, Chamada FAPESP-ANR-2021 - MagGlass (Université Bordeaux França) - R$ 600,000,00 (Submitted)
M. NALIN, Chamada Sisfóton MCTI-CNPq -2021 - 460.000,00
A.C.M. RODRIGUES- ICG - International Commission on Glass - Euro 2,000 Jan. 2019-Sept. 2021

Prestigious CNPq fellowships/grants to the CeRTEV faculty

ECKERT, H., Bolsa CNPq, Nível 1A, (renovado, 2021-2025)
ZANOTTO, E.D., Bolsa CNPq, Nível 1A
PIZANI, P.S., Bolsa CNPq, Nível 1B

RINO, J.P. Bolsa CNPq, Nível 1B
MASTELARO, V.R., Bolsa CNPq, Nível 1B
DE CAMARGO, A. S. S., Bolsa CNPq, Nível 1D
SCHNEIDER, J., Bolsa CNPq Nível 2
DONOSO J.P., Bolsa CNPq Nível 2
NALIN, M., Bolsa CNPq Nível 2
RODRIGUES A.C.M. Bolsa CNPq, Nível 1D (renovada 2021-2023)

Overall budget of the Center from other sources, July 2019- June 2020

Funded Projects by CAPES and CNPq	R$ 582.500
International funds including student fellowships	Euro 166.750
CNPq Fellowships (bolsas) to CeRTEV professors	R$ 236.400
Student IC, MSc, Dr, PD / grants from all sources	R$ 850.000
Grants from companies	Euro 382.000
Professor´s salaries USP, UFSCar, UNESP	R$ 3.178.000
Staff salaries UFSCar, USP	R$ 600.000

*1 US$ ~ 5R$ ~ 0.85 Euro

Contracts celebrated with international institutions

- Rodrigues, Council of Scientific & Industrial Research (CSIR) and Central Glass & Ceramic Research Institute (CSIR-CGCRI), India
- Rodrigues, Zanotto, Peitl, Andreeta - Clausthal University, Germany
- Rodrigues, Zanotto, Institut de Physique du Globe de Paris, France
- Rodrigues, A.C.M.R., Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB - UMR 9048), Centre National de la Recherche Scientifique, The University of Bordeaux, The Polytechnical Institute of Bordeaux
- Zanotto - CeRTEV with FunGlass Institute, European Union
- Eckert, Westfälische Wilhelms Universität Münster, Germany
- Eckert, Shanghai Institute of Optics and Fine Mechanics (SIOM), China
- Eckert, University Rennes, University Montpellier, TU Munich, LMU Munich, University of Torino, University of Poznan, (EU-MaMaSELF)
- Nalin, Instituto de Química- DAFQI-UNESP - Universidade de Bordeaux, França- Université de Bordeaux- Lionel Canioni -FUNGlass H2020-MSCA-RISE-2018
- Nalin, França - Université de Bordeaux - Thierry Cardinal - Photonics International network - PIN - CAPES-PRINT-Unesp
-Nalin, Instituto de Química- DQGI-UNESP - Universidade de Laval - Quebec Canadá - JIRU (Joint International Research Unit)
-De Camargo, Instituto de Física - WWU Muenster e Fundação Alexander von Humboldt, Bart Jan Ravoo, Alemanha

- Pizani, PS, Université de Lyon, BEPE FAPESP Proc. 2019/11446-6

GENERAL SCIENTOMETRIC INFORMATION

81 glass-related articles have been published in scientific journals in the period, most of them by the PIs. They are listed in the end of this report. Also, 28 other papers related to crystalline materials and liquids have been published by the CeRTEV faculty.

All the CeRTEV publications on vitreous materials on Google Scholar since 2013, updated May 30, 2021 are listed in the following link:

CERTEV-GLASS LAMAV - Google Acadêmico

Summary Jan. 2013 to May 30, 2021
CeRTEV h=38, i10 = 168; citations 5,500.

Highlighted articles in 2019 and 2020
*Invited by editors, highly cited, most downloaded, awarded prizes, attracted media attention, etc.

MOST DOWNLOADED JNCS ARTICLES IN 2020 (among ~27,500 Articles)

Downloads in 2020	**Downloads lifetime**	**Article Title**	**Authors**	**Publication Year**
733 1rst	11,523	Updated definition of glass-ceramics	**Deubener J., Davis M.J., Komatsu T., Nakane S., Zanotto E.D.,** et al.	2018
246 6th	11,456	The glassy state of matter: Its definition and ultimate fate	**Zanotto E.D.,** Mauro J.C.	2017
259 5th	5,695	Biosilicate® - A multipurpose, highly bioactive glass-ceramic.	Crovace M.C., Souza M.T., Chinaglia C.R., **Peitl O., Zanotto E.D.**	2016

*Names in **bold** = CeRTEV Professors or IAB members

MOST CITED JNCS ARTICLES IN 2020 (Published IF Window 2017-2018)

Citations In 2020	**Total Citations**	**Article Title**	**Authors**	**Year**
39 (2th)	71 since 2018	Updated definition of glass-ceramics	**Deubener J., Davis M.J., Komatsu T., Nakane S., Zanotto E.D.,** et al.	2018

*Names in **bold** = CeRTEV Professors or IAB members

JOHN C. MAURO and EDGAR D. ZANOTTO - Two Centuries of Glass Research: Historical Trends, Current Status, and Grand Challenges for the Future - International Journal of Applied Glass Science Pages: 313-327, Published: 28 July 2014 (Most read in 2019, 2nd place - most read article ever, 4th most read in 2020)

Examples of CeRTEV in the media in the period July 2020-June 2021

COVID actions

- (16) #VacinaSim | Edgar Dutra Zanotto - YouTube
- Vídeo compara, erroneamente, pesquisadores que estudam covid-19 (estadao.com.br)

- My Fulbright experience in Brazil: a wonderful journey on glass research and cultural exchanges | The American Ceramic Society
- Sob medida – ABC
- Em busca de métricas mais refinadas : Revista Pesquisa Fapesp
- Edgar Zanotto conversa sobre seu estudo pioneiro no uso de IA para o desenvolvimento de materiais vítreos | by Vanessa Petuco | Aprix Journal | Mar, 2021 | Medium
- Tirinhas divulgam conhecimento e curiosidades sobre vidros - São Carlos Agora (saocarlosagora.com.br)
- Professores da USP São Carlos e UFSCar juntos em Feira Virtual de Ciência e Tecnologia - São Carlos Agora (saocarlosagora.com.br)
- Edgar Dutra Zanotto, PhD - Editors - Journal of Non-Crystalline Solids (elsevier.com)
- ‘Tirinhas de Vidro’ mostram diversidade de materiais vítreos | IMPA - Instituto de Matemática Pura e Aplicada
- Lista de cientistas mais influentes do mundo conta com 15 membros da ANE - Academia Nacional de Engenharia (anebrasil.org.br)
- Professores da UFSCar integram lista de cientistas mais influentes do mundo | São Carlos em Rede (saocarlosemrede.com.br)
- Biosilicato — Português (Brasil) (ufscar.br)
- 2nd (ICAIC) International Conference for Academia and Industry Co-operation & 2nd (IMMSEM) International Meeting in Materials Science and Engineering of Maranhão (even3.com.br)
- Vidraçaria São Paulo - Curiosidade (vidracariasaopaulo.com.br)
- Eleita a Nova Diretoria e Membros do Conselho – Gestão 2021 e 2022 – ABCERAM
- https://g1.globo.com/sp/sao-carlos-regiao/noticia/2021/03/22/instituto-de-quimica-da-unesp-de-araraquara-cria-sensor-que-detecta-antibiotico-em-esgotos.ghtml
- https://www.iq.unesp.br/#!/noticia/737/unesp-cria-sensor-para-detectar-antibiotico-em-rios-e-esgotos
- https://www.cbnararaquara.com.br/noticias/SOM,0,0,74002,Cientistas+da+Unesp+criam+sensor+que+detecta+antibioticos+em+rios+e+esgotos.aspx
- https://www.cbnararaquara.com.br/noticias/SOM,0,0,79068,Qual+a+importancia+da+luz+para+a+ciencia.aspx

- https://namidia.fapesp.br/a-cidade-on-sao-carlos-sp/13792
- https://youtu.be/V1MDkufnVEU
- https://www2.ufscar.br/noticia?codigo=13847

TALKS AT INTERNATIONAL CONGRESSES, WORKSHOPS, AND SYMPOSIA July 2020 - June 2021

-DE CAMARGO, A. S. S. - Exzellenz verbindet – be part of a worldwide network, GYA WEBINAR – Empowering Women in Science, India, July 2020, INVITED (online).
-DE CAMARGO, A. S. S. - Exzellenz verbindet – be part of the worldwide AvH network, WWU Muenster Alumni Meeting, Germany, November 2020, INVITED (online).
-DE CAMARGO, A. S. S. - From lighting devices to photodynamic therapy: Contributions from LEMAF for the development of photonic and biophotonic materials, WFWIS – World Forum for Women in Science, Iraq, March 2021, INVITED (online).
-DE CAMARGO, A. S. S. - Gender Equality in Sciences: Let's teach our girls to be brave, Humboldt Virtual Networking Event "Early career researchers wanted! Chile´s next generation of humboldtians, Chile, April 2021, INVITED (online).
-DE CAMARGO, A. S. S. - Solar light mediated photodynamic water disinfection through low-cost biomass nanocomposites, ACS 25th Annual Green Chemistry and Engineering Conference, USA, June 2021, INVITED (online).

-ZANOTTO E.D. - Pitfalls and successes of the CNT – PANNANO Pan American Meeting on Nanomaterials - Águas de Lindoia - March PLENARY (presential).
-ZANOTTO E.D.- Glass greats – Penn State Meeting of Young Researchers- State College, USA – July PLENARY (online).
-ZANOTTO E.D. – four international talks cancelled due to the COVID.

-ECKERT H. - New Magnetic Resonance Strategies for Studying Structure/Property correlations in Laser Glasses, ICONS (Intercontinental Seminars) 2020, September 2020 INVITED (online).
-ECKERT, H. - The Glassy Part of Glass-Ceramics, Symposium of Solid-State NMR on Inorganic Materials, INVITED, American Chemical Society Spring Meeting, April 2021 (online).

NATIONAL MEETINGS July 2020 – June 2021

DE CAMARGO, A. S. S. - A excelência conecta – faça parte da rede global da Fundação AvH, Mesa Redonda: Alemanha – Perspectivas e Oportunidades, SIA 2020 – Simpósio de Integração Acadêmica Universidade Federal de Viçosa, Viçosa - MG, July 2020, INVITED (online).
DE CAMARGO, A. S. S. - Exzellenz verbindet – be part of the worldwide AvH network, Webinar Oportunidades para Pós Docs, São Paulo - SP, September 2020, INVITED (online).
DE CAMARGO, A. S. S. - Híbridos hóspede-hospedeiros e sistemas nanoparticulados para aplicações fotônicas e biofotônicas, Colóquio no Instituto de Física da UFPE, Recife - PE, September 2020, INVITED (online).

DE CAMARGO, A. S. S. - Bem-vindos à era do Vidro, Ciclo de webinários da Pós-graduação em Química e Ciências dos Materiais da Universidade Federal do Mato Grosso do Sul, Dourados – MS, October 2020, INVITED (online).
DE CAMARGO, A. S. S. - Panorama da Participação das Mulheres nas Ciências Exatas, XVI Semana da Física da UFSCar, São Carlos – SP, October 2020, INVITED (online).
DE CAMARGO, A. S. S. - 90% das cientistas premiadas do país relatam machismo, Article in the Jornal Estadão, São Paulo – SP, October 2020, INTERVIEW https://istoe.com.br/90-das-cientistas-premiadas-do-brasil-relatam-machismo/
DE CAMARGO, A. S. S. - Rare Earth doped oxide and oxyfluoride scintillating glasses, EOSBF 2020 – Encontro de Outono da Sociedade Brasileira de Física, November 2020 (online).
DE CAMARGO, A. S. S. - Mulheres nas Ciências, Jornal da Tarde da TV Cultura, São Paulo – SP, November 2020, INTERVIEW.
https://www.youtube.com/watch?v=K2j4_vlmwKU
DE CAMARGO, A. S. S. - A excelência conecta – Faça parte da rede internacional Alexander von Humboldt, Seminário de Pós-Graduação do DF/UFSCar, São Carlos – SP, March 2021, INVITED (online).
DE CAMARGO, A. S. S. - Novo método de descontaminação de água alia compósitos de baixo custo e energia solar, Agência FAPESP, São Paulo – SP, March 2021 https://agencia.fapesp.br/novo-metodo-de-descontaminacao-de-agua-alia-compositos-de-baixo-custo-e-energia-solar/35487/.
DE CAMARGO, A. S. S. - Novo método para descontaminação de água, Rádio Nacional, Brasília – DF, April 2021, INTERVIEW: https://radios.ebc.com.br/tarde-nacional/2021/04/pesquisadores-desenvolvem-metodo-para-descontaminacao-da-agua.
DE CAMARGO, A. S. S. - Descontaminação da água que usa compostos de baixo custo e energia solar, Programa ALESP conecta (Jornalista July Stanzioni), YouTube, May 2021, INTERVIEW: https://www.youtube.com/watch?v=Rale_cYOx-U.
DE CAMARGO, A. S. S. - Mulheres na Ciência, Fala PET IQSC/USP #3, Canal YouTube, May 2021, DEBATE: https://youtu.be/Nub3J0z2Uak.
DE CAMARGO, A. S. S. - Bem vindo a Era do Vidro, Video Mulheres na Ciência #98, YouTube, May 2021. https://youtu.be/s0haxolROCQ.
DE CAMARGO, A. S. S. - Development of novel rare-earth doped scintillating glasses and glass-ceramics, EOSBF 2021 – Encontro de Outono da Sociedade Brasileira de Física, June 2021 (online).

ZANOTTO E.D. - Benvindo à Era do Vidro – UFGC, Paraíba, June - PLENARY (online) 2020.
ZANOTTO, E.D. - talk of 2019 that was not included in the previous report (24) I SPIMF - Edgar Dutra Zanotto - YouTube.
ZANOTTO E.D.- Machine learning guided design of glasses – 17ª Semana Nacional de C e T – October, PLENARY (online) - (24) 17a. SNCT: Palestras - Segunda-feira 19/10 - YouTube .
ZANOTTO E.D. - Design of vitreous and crystalline materials via AI – SEMMAT 2020-October, UFF, PLENARY (online).
ZANOTTO, E.D. Palestra II SerCET - (24) II SerCET - Módulo 1: Conteúdos e Aplicações do Ensino Remoto nas Engenharias e Exatas - YouTube
ZANOTTO E.D. Talk IT Maranhao.

Conferences, workshops, and symposia organized or co-organized by Certevians

E.D. ZANOTTO - Glass and Optical Materials Meeting 2020 – Crystallization session (chairman) - American Ceramic Society. August 2020.
DE CAMARGO, A. S. S. - Sessão de Óptica e Fotônica - EOSBF 2020 – Encontro de Outono da Sociedade Brasileira de Física (organizadora). November 2020.

Awards and distinctions granted to CeRTEV faculty in the period July 2020- June 2021

ECKERT, H. - **Hellmut Eckert Festschrift**. Virtual Special Issue of the Journal of Physical Chemistry C, Vol. 125, May 2021. Career achievement award, featuring 53 dedicated scientific articles, autobiography, salutation, c.v., list of publications, and collaborators.

ECKERT, H.; MASTELARO V.R., and ZANOTTO, E.D.- Ranked among the **2% most impactful** scientists of all areas in 2019, and all times (ECKERT and ZANOTTO), PLOS-Stanford rank October 2020.

ZANOTTO, E.D. et al. - Three articles ranked among the **7 most downloaded** and one most cited of the JNCS in 2020 – "Updated definition of glass-ceramics" (published in 2018), Elsevier.

ANDREETA, M. R. B. - Cover of the Crystal Growth & Design Journal, May issue 2021.

DE CAMARGO, A. S. S., Physics Opinion (American Physics Society): "Positives from Online Teaching", Ed. Jessica Thomas, Physics 13(130), August 2020. https://physics.aps.org/articles/v13/130

DE CAMARGO, A. S. S., Back cover Highlight, *Porosity induced rigidochromism in platinum (II) terpyridyl luminophores @ silica composites*, A. E. Norton, K. P. S. Zanoni, M.-A. Dourges, L. P. Ravaro, M. K. Abdolmaleki, A. S. S. de Camargo, T. Toupance, W. B. Connick, S. Chatterjee, J. Phys. Chem. C 9 (2021) 6193-6207.

Short courses delivered in the period

H. ECKERT, Rotational Echo Double Resonance in Solid State NMR: Theoretical and Practical Aspects, IBqM graduate program, UFRJ, Brazil, March 2021.
H. ECKERT, Workshop on Solid State NMR, MaMaSELF Program, University of Montpellier, France, April 2021.
H. ECKERT, Master Course in Spectroscopy and Structure of Matter, University of Münster, Germany, June 2021.
ZANOTTO, E.D. - Fundamentals and applications of glass crystallization - American Ceramic Society, August 2020.

Editorship of scientific journals in 2019-2020

DE CAMARGO, A. S. S. - Editor of the Journal of Materials Science (Springer Nature) since

2021.

RODRIGUES, A.C.M. - *Associate Editor*, Frontiers in Materials: Glass Science.

ECKERT, H. - *Editorial Board Member*, Solid State Nuclear Magnetic Resonance (Elsevier).
ECKERT, H. - *Editorial Board Member*, Zeitschrift für Naturforschung, (Physics), de Gruyter.

ANDREETA, M.R.B. - *Associate Editor*: Open Chemistry Journal (ISSN: 1874-8422).
ANDREETA, M.R.B. - *Editorial Board Member*, EUREKA: Physics and Engineering (ISSN 2461-4254 (Print)).

MASTELARO, V. - *Member of the Editorial Commission of Materials Research:* Ibero-american Journal of Materials.
MASTELARO, V. - *Associate Editor:* Journal of Alloys and Compounds (Elsevier).

ZANOTTO, E. D. - *Editor* of the Journal of Non-Crystalline Solids since 2010.
ZANOTTO, E. D. - International Materials Reviews (UK) - *Key Reader* and Board member.
ZANOTTO, E. D. - *Member of the International Advisory Boards of 9 other journals:* Springer-Nature Applied Sciences (UK), Materials (Switzerland), International Journal of Applied Glass Science (USA), Materials Research (Ibero-American), Biomedical Glasses (Germany)- discontinued in 2021, Iranian Journal of Materials Science and Engineering (Iran), Bulletin de la Sociedad Espanhola de Ceramica y Vidrio (Spain), Results in Physics (Argentine), Cerâmica (Brazil).

International standing of CeRTEV faculty and board members on the Stanford-PLOS ranking 2020

by Edgar D. Zanotto, Karina Lupetti and Hellmut Eckert

There is no absolute quantitative parameter accepted worldwide to assess a scientist's work quality, but there are relevant indicators. A key question refers to the major scientific or technological discoveries of the researcher.

Relevant articles describing new discoveries often result in invited and plenary conference talks, prizes bestowed by scientific organizations, and substantial increases in research funding. They also tend to increase the awardee's responsibilities to his/her scientific community, including invitations to join science academies, to serve as an editor for scientific journals, or to serve on review boards making funding, awards or career promotion decisions. All of these honors, accomplishments, and responsibilities reflect the respect among peers for scientist´s contributions to science, technology or society. Combining such pieces of information can provide a revealing overview of the quality of a researcher's work [Zanotto - Scientometrics 2006]. However, it can become a gigantic, unpractical task when a selection within a large group of applicants has to be made. This includes picking a winner among hundreds of candidates for a prize or a seat in a science academy, making a funding decision in a competition for a research grant, or choosing the site of a new research center.

In this context, in the last three decades, bibliometric indexes have emerged, which account for published articles and citations received by them in different ways. While they do not provide a direct measure of quality, in principle, some of these parameters can reveal the prolificity, visibility, and impact of an author or group by their peers [Montazerian, Zanotto & Eckert 2019, 2020], [Montazerian, M., Zanotto, E.D., Eckert, H. (2017) International Journal of Applied Glass Science.] As most of these indexes increase with the number of published articles, and also are highly dependent on the area of research, a direct comparison of individuals is not possible, neither between authors of different age groups, nor between authors working in different research fields. But the scientometry has evolved; since the appearance of the H-index more than a hundred impact parameters have been proposed, and some of them, in some way (not yet wholly satisfactory) normalize citations and publications by the age of the article and area of knowledge, e.g. [Montazerian, Zanotto & Eckert – Scientometrics 2019, 2020]. [Zanotto & Carvalho - Scientometrics 2021].
Recently, a renowned group from Stanford University [Ioannidis, Boyack, Baas - PLOS Biology, 2016, 2019, 2020] has used a more complete indicator, combining 12 parameters, and published a ranking of approximately 160,000 scientists that were considered the most influential on the planet, taking into account their impact and international visibility. These selected researchers compose approximately 2% of the universe of more than 7 million scientists analyzed [Ioannidis, Boyack, Baas - PLOS Biology 2020]. The Stanford group analyzed the bibliometric performance of all authors with more than 5 articles indexed by Scopus since 1960; a Herculean work, which provides the most complete panoramic view ever carried out in the area of scientometry.

The formula for calculating this index [John Ioannidis, Kevin W. Boyack and Jeroen Baas - PLOS Biology, 2016, 2019, 2020] takes into account parameters that reflect publications since 1960 and citations of these researchers accumulated throughout their careers. A second index is also presented, referring to all articles published, but analyzing their citation statistics in the year 2019 alone. While both indexes tend to favor prolific senior researchers, the 2019 index may be viewed as a better reflection of the current relevance of a scientist's accumulated work. The bibliometric data are tabulated and two alternate versions can be consulted on the journal's website, taking self-citations into account or not. Based on this spreadsheet, we performed an analysis of glass researchers, which is presented here.

Regarding inorganic, non-metallic vitreous materials, more than 80 scientists from 23 countries appear within the 2% most impactful in 2019 for their contributions throughout their career, starting in 1960. We only spotted the glass researchers that appear in the Scopus list of the 100 most prolific (published the largest number of articles) with the keyword "glass*", excluding metallic and organic glasses, hence several might be on the Stanford list but were not detected by our search of a few needles in the haystack. This was not a complete quest; the idea was to test whether and to which extent glass science could make it in this ranking of all scientific fields.

Four of the spotted glass scientists are ranked among the first 2,000, and at least fifteen among the 20,000 most influential scientists (according to citations in 2019); with the

great Larry Hench* (r= 469th) and Austen Angell* (r= 619th) among the top 1,000 most visible scientists of all areas! These results support our opinion that these two distinguished individuals are among the most influential glass scientists of all times; hence their positions in this ranking corroborate the perception of the glass research community. While this list shows the most impactful scientists, we stress again that it tends to favor the most prolific and most senior scientists, having accumulated large numbers of papers over many years. Owing to its construction, it cannot account adequately for the contributions of younger scientists, regardless of the quality of their articles.
*deceased

We computed the relative positions of the most prolific glass researchers in the Stanford-PLOS ranking. The principal conclusions are the following:
(1) Approximately 80-100 researchers from the area of glass science are represented in this ranking of top 2% researchers, indicating that this research area is very active, arousing a great deal of scientific interest,
(2) Two CeRTEV principal investigators (Zanotto and Eckert) and thirteen members of the international scientific advisory board appear in the lists.
(3) The overwhelming majority of the individuals are present on both lists, but a few younger authors only appear in the 2019 list, whereas some elderly researchers only appear in the whole career listing. These findings are consistent with the general perception that impact research in glass science tends to be built upon the accumulated scientific progress created by the consistent and long-term commitment of its scientists.

There is a loose estimate that approximately 3,000 glass scientists and technologists are active. In the Ioannides et al. universe of 7.5M researchers, we represent only 0.04% of the total. With ~80 glass researchers in the 160.000 list, we are 0.05%, which is proportional to the number of active glass researchers.

The main conclusion of this contribution is the fact that among the scientists of the 174 different disciplines analyzed, glass scientists are reasonably represented in the list of the 160,000 most influential individuals. On the other hand, it is obvious that the Stanford ranking privileges senior researchers who initiated their careers several decades ago. It also includes deceased scientists. As such, the index does not give sufficient credit to the (more recent) accomplishments of young and mid-career scientists. An alternative useful indicator could be obtained by limiting the citation analysis to the work published by researchers over a more limited time, for example the most recent 20 years. This may be more suitable criteria for reaching funding decisions in competitions for research grants. Summarizng, while it does not measure research quality and is certainly not the ultimate measure of visibility and impact, this is indeed the most complete scientometric study ever conducted and showcases the **international standing of the CerTEV researchers and board members.**

References

-IOANNIDIS, J.P.A., BAAS, J., BOYACK, K.W. -Updated science-wide author databases of standardized citation indicators (2020) PLoS Biology, 18 (10), art. no. e3000918,

-IOANNIDIS, J.P.A., BAAS, J., KLAVANS, R., BOYACK, K.W.- A standardized citation metrics author database annotated for scientific field (2019) PLoS Biology, 17 (8), art. no. e3000384,
-IONNIDES, J.P.A., KLAVANS, R., BOYACK, K.W., Multiple Citation Indicators and Their Composite across Scientific Disciplines (2016) PLoS Biology, 14 (7), art. no. e1002501.
-MONTAZERIAN, M., ZANOTTO, E.D., ECKERT, H.-Prolificacy and visibility versus reputation in the hard sciences (2020) Scientometrics, 123 (1), pp. 207-221.
-MONTAZERIAN, M., ZANOTTO, E.D., ECKERT, H.-A new parameter for (normalized) evaluation of H-index: countries as a case study (2019) Scientometrics, 118 (3), pp. 1065-1078.
-MONTAZERIAN, M., ZANOTTO, E.D., ECKERT, H. - Bibliometrics in glass and other sciences: A Plea for reason (2017) International Journal of Applied Glass Science, 8 (3), pp. 352-359.
-ZANOTTO, E.D., CARVALHO, V., Article age- and field-normalized tools to evaluate scientific impact and momentum (2021) Scientometrics, 2021.
-ZANOTTO, E.D., The scientists pyramid (2006) Scientometrics, 69 (1), pp. 175-181.

Administrative and consulting role in scientific societies in 2020 – 2021

DE CAMARGO, A. S. S. – *Membro do Conselho*, Clube Humboldt do Brasil, desde 2014.
DE CAMARGO, A. S. S. *Diretora Científica da SBPMat* - since February 2020.
DE CAMARGO, A.S.S. *Brazilian Ambassador Scientist,* Fundação Alexander von Humboldt, since July 2020.
MASTELARO, V.R. *Conselheiro Titular* da SBPMat de 2020 a 2024.
RODRIGUES, A.C.M. – *Chair* of the ICG TC23: Education in Glass.
NALIN, M. - *Member* of the ICG TC20: Optoelectronics.
FERREIRA, E. B. – *Glass Committee* of the Brazilian Ceramic Society.
ECKERT, H. - *Advisory Board member*, Network of the French High-Field NMR Facilities.
ECKERT, H. – *Hans - Hellmuth Vits-Prize Committee*, Society of the WWU Münster.
ECKERT, H. - *Member, Board of Coordinators*, Physics, FAPESP.
ZANOTTO, E.D. - *President of the Curators Council* of the São Carlos TechPark.
ZANOTTO, E.D. - *Board of Directors of the Brazilian* Ceramic Society.
ZANOTTO, E.D. - *Brazilian representative* in the International Commission on Glass.
ZANOTTO, E.D. - *Council member* of the International Ceramic Federation.
ZANOTTO, E.D. - *Council member* of the FunGlass Institute, European Union.
ZANOTTO, E.D. - *Board member* of the Serrapilheira (Funding) Institute.
ZANOTTO, E.D. - *Board member* of IMPA (Institute of Mathematics), Brazil.
ZANOTTO, E.D. - *Member of the Glass Crystallization / GC Committee*: ICG TC07.
ZANOTTO, E.D. - *Engineering Fellowship Selection Committee*, TWAS.
ZANOTTO, E.D. - *Gottardi Prize*, Voting Member, ICG.
ZANOTTO, E.D. - *Zachariasen and Mott Awards*, Selection Committee, JNCS.
ZANOTTO, E.D. - 4 prizes EPDC Committee, American Ceramic Society.
ZANOTTO, E.D. - *CBMM Prize Selection Committee*, CBMM, Brazil.
ZANOTTO, E.D. - *Sao Carlos Scientist of the Year Award Committee*, São Carlos, Brazil.
ZANOTTO, E.D. - Brazilian Academy of Sciences WG for reformulation of the CNPq productivity award grants.

International visitors in 2020-2021 (covid year)

Dr. Vladimir Fokin- St. Petersburg (FERREIRA & ZANOTTO).

Voluntary activities within the respective universities

DE CAMARGO, A. S. S. - Vice-Presidente Comissão de Pesquisa IFSC - 05/16 – atual.
DE CAMARGO, A. S. S. - Membro titular da Comissão de Pós Graduação Ciência e Engenharia de Materiais, EESC/USP - 08/14 – atual.
DE CAMARGO, A. S. S. - Membro titular da Comissão Coordenadora do Curso de Bacharelado em Química, IQSC/USP - 03/17 – atual.
DE CAMARGO, A. S. S. - Membro titular do Conselho de Depto. Física e Ciência Interdisciplinar, IFSC/USP – Maio/16 – atual.
DE CAMARGO, A. S. S. - Membro titular da Congregação do IFSC/USP, IFSC/USP – 08/16 - atual.
DE CAMARGO, A. S. S. - Membro da Comissão de Assessoramento da Chefia do Dept. de Física e Ciência Interdisciplinar e da Diretoria para distribuição de espaço físico (2019).
DE CAMARGO, A. S. S. - Membro da Comissão de Assessoramento da Chefia do Dept. de Física e Ciência Interdisciplinar para elaboração do plano institucional departamental 2018-2023.

ECKERT, H. – Membro titular de Comissão Relações Internacionais (CRINT).
ECKERT, H.- Membro titular do Conselho de Depto. Física e Ciência Interdisciplinar, IFSC/USP.
ECKERT, H. - Membro titular da congregação do Instituto de Física São Carlos (IFSC), USP.
ECKERT, H. - Membro titular da Comissão de Progressão Horizontal da Carreira Docente, (IFSC), USP.

NALIN, M - Vice-Chefe do Departamento de Química Analítica, Físico-Química e Inorgânica, IQ-Unesp, Araraquara (2020-2021).

FERREIRA, E.B. - Membro Titular do Conselho do Departamento de Engenharia de Materiais, EESC/USP, 2018 – atual.
FERREIRA, E. B. – Suplente da Comissão de Pesquisa, EESC/USP, 2017 – Atual.
FERREIRA, E. B. – Membro suplente da Comissão Coordenadora do Curso de Engenharia de Materiais, EESC/USP, 2018 – atual.

ANDREETA, M. R. B. - Coordenador da atividade de extensão ACIEPE - "Engenheiros e Cientistas do Futuro" dedicada à difusão do conhecimento científico.
ANDREETA, M. R. B. - Vice-coordenador da área de Materiais Cerâmicos- DEMa -UFSCar (6/2019 - 11/2020).
ANDREETA, M. R. B. - Suplente do Conselho Departamental do DEMa/UFSCar (6/2019 - 11/2020).
ANDREETA, M. R. B. - Coordenador da área de Materiais Cerâmicos- DEMa -UFSCar (11/2019 - 5/2020).
ANDREETA, M. R. B. - Membro titular do Conselho Departamental do DEMa/UFSCar (11/2019 - 5/2020).

ANDREETA, M. R. B. - Vice-coordenador da área de Materiais Cerâmicos- DEMa -UFSCar (5/2021 - 5/2022).
ANDREETA, M. R. B. - Suplente do Conselho Departamental do DEMa/UFSCar (5/2021 - 11/2022).
ANDREETA, M. R. B. - Membro suplente da Coordenadoria de Iniciação Científica e Tecnológica (CCET Tecnológicas - Campus São Carlos) - 2020/2022.

SCHNEIDER, J.F. – Coordenador do Curso de Bacharelado em Física, Instituto de Física de São Carlos/USP, 2016 – atual.
SCHNEIDER, J.F. – Membro da Comissão de Graduação, Instituto de Física de São Carlos/USP, 2016 – atual.
SCHNEIDER, J.F. – Membro da Comissão de Cooperação Internacional, Instituto de Física de São Carlos/USP, 2021 – atual.

ZANOTTO, E.D. - Member of the committee for evaluation of faculty performance, PPGCEM/ UFSCar, 2015 – Present.
ZANOTTO, E.D. - Supervisor of the LaMaV / UFSCar since 1977.

RINO, J.P. – Membro titular representante do CCET para avaliação e desempenho acadêmico dos docentes. 2015-2019.
MASTELARO VR- Membro Titular junto ao Conselho Departamental FCM desde 04.02.2010.
MASTELARO VR- Chefe do Departamento de Física e Ciências dos Materiais desde 2020-2022.
MASTELARO VR- Membro Titular junto a congregação do IFSC desde 05/.2018.
DONOSO, G.J. - Membro da Comissão de Cultura e Extensão, IFSC - USP (desde 2018).

Current Research Students and Post-docs working on glasses and vitreous materials July 2020 – June 2021

Current internship (IC) students working on vitreous materials			
Edgar Dutra Zanotto			
Enzo Miguel	IC	2019 - 2021	FAPESP
Eduardo Bellini Ferreira			
Icaro Marino Bittencourt (with C. Magon)	IC	2020-2021	FAPESP (cota)
Letícia Cursini	IC	2019-2020	FAPESP (cota)
		2017-2019	PUB-USP
Marcelo Nalin			

Victoria Luisa Mameli	IC	2020-2021	PIBIC
Nicole Roque	IC	2020-2021	VUNESP
Marcello R. B. Andreeta			
Marcelo Watanabe Machado	IC	2021-2022	FAPESP/PIBIC
Andrea S. S. de Camargo			
Gabriel Brambilla	IC	2019-2020	PIBIC
José Pedro Donoso Gonzalez			
Flavio Alves Conti	TCC	2020	w/o fellowship
Hellmut Eckert			
Victor Reis	IC	2020	w/o fellowship

Current MSc and PhD students working on vitreous materials			
Edgar Dutra Zanotto			
Maurício Lima	MSc	2020-2022	CNPq
Ricardo F. Lancelotti	PhD	2021-2023	FAPESP
Andreia de Menezes	MSc	2020-2021	CBMM
Rodrigo C. Passos	MSc	2019-2021	FAPESP
Maria H. Acosta (Colombia)	PhD	2017-2021	CNPq
Débora Fabris	PhD	2017-2021	CAPES
Bruna Valerini (w/ Odonto-UNESP)	PhD	2019-2022	CNPq
Lorena Rodrigues	PhD	2018-2021	CNPq
Thalia Delmondes	MSc	2020-2022	CNPq
Andrea de Camargo			
Raquel Riciatti do Couto Vilela	PhD	2017-2021	CAPES
Thiago Augusto Lodi	PhD	2018-2022	CNPq
Walter Justi Faria	PhD	2019-2023	CNPq
Marylyn Setsuko Arai	PhD	2019-2023	CNPq
Vitor de Lima Reis	MSc	2020-2022	CNPq

Pedro Martins Garcia da Costa	PhD	2020-2024	FAPESP
Eduardo Bellini Ferreira			
Katherine Santos Oliveira	MSc	2019-2021	CAPES
João Matheus Rugeri Murdiga	MSc	2019-2021	CAPES
Mariana Cristina Haleplian Pinto	MSc	2018-2021	Glass company
Flávio Vilas Boas	MSc	2019-2022	-
Ana Caroline Batista Pires	MSc	2020-2022	CAPES
Guilherme Silva Macena	PhD	2019-2023	CAPES
Johnata Cavalcanti Fonseca	PhD	2019-2023	CAPES
Karem Janeth Rimachi Hidalgo (Peru), (coorientação Odonto UNESP)	PhD	2018-2022	CAPES Institucional (até Dez/2019)
Marcello R. B. Andreeta			
Armando José de Sá Santos	MSc	2020-2022	w/o fellowship
Stevenson Pierre Louis	MSc	2020-2022	w/o fellowship
Marcela Edith Figueroa Arteaga	MSc	2020-2022	w/o fellowship
Flavia Bueno Mendes	MSc	2020-2022	w/o fellowship
Eliandro Pereira Teles	MSc	2020-2022	sem bolsa
Maíra Dombroski Neme	MSc	2019-2021	CNPq
Natã Pereira de Almeida	PhD	2019- 2023	CNPq
Ana Candida M. Rodrigues			
Vinicius Martins Zallocco	MSc	2019-2021	CNPq
Lucas Hidalgo Pitaluga	MSc	2020-2022	SCHOTT Brasil
Felipe Barros Lacaz	MSc	2020-2021	w/o fellowship
Paulo Sergio Pizani			
Rafaella Bartz Pena	PhD	2017-2022	FAPESP
José F. Schneider			
Gabriel Felipe Morguetto	PhD	2020-2024	CAPES
Hellmut Eckert			

Hugo Damasceno	MSc	2017-2021	Nippon Glass
Millena Logrado	PhD	201 -2021	Nippon Glass
Marcelo Nalin			
Leonardo V. Albino	PhD	2019-2022	CAPES
Samira N. Stain	PhD	2019-2022	CAPES
Juliana Moreno Paiva	PhD	2018-2021	CAPES
Valmor R. Mastelaro			
Vinicius Duarte Jesus	MSc	2019-2021	CAPES
Valdinei Liber	MSc	2020-2022	CNPq

Current Post-Docs working on vitreous materials (grant good up to)		
Edgar Dutra Zanotto		
Leila Separdar (Iran) w/ Rino	FAPESP	Aug. 2019 - 2022
Azat Tipeev (Russia) w/Rino	FAPESP	2019 - 2022
Gisele Guimarães	AGC, Japan	May 2019 - Oct. 2021
Daniel Roberto Cassar	FAPESP	2017- June 21
Henrik Bradtmueller (Germany) w/ Hellmut	FAPESP	Nov. 2020-2022
Marina T. Souza	Vetra, Brazil	Dec. 2021
Laís Dantas	IVOCLAR AG, Liechteinstein	2019 - Feb. 2022
Viviane Oliveira Soares	CNPq	2019 - 2021
Rafael Bonacim de Oliveira	CBMM, Brazil	Dec. 2021
Claudia Abadia (Colombia)	CAPES	2021-2022
Hellmut Eckert		
Bianca Cerrutti	Sem bolsa	Dec. 2021
Igor Danciaes	FAPESP	May 2021
Henrik Bradtmüller	WWU Münster	Oct. 2020
Andrea S.S. de Camargo		

Gustavo Galleani	FAPESP	2020
Leonnam Gotardo Merizio	FAPESP	2020
José Pedro Rino		
Azat Tipeev (Russia) (w/Zanotto)	FAPESP	2021
Leila Separdar (Iran) (w/Zanotto)	FAPESP	Aug. 2019 - 22
Ana Candida Martins Rodrigues		
Nilanjana Shasmal (Índia)	FAPESP	Renewal submitted
Adriana Yumi Iwata	FAPESP/Jornalismo	2020-2021
Paulo Sérgio Pizani		
Benjamin Moulton (Canadá)	FAPESP	2021
Thiago Rodrigues da Cunha	FAPESP	Cota FAPESP
Marcelo Nalin		
Douglas Faza Franco	FAPESP	2018-2021
Lia Mara Marcondes	FAPESP	2021-2023
Juliane Resges Orives	FAPESP	2019-2022-Cota FAPESP
Eduardo Bellini Ferreira		
Maria Costa (w/ *Eckert*)	FAPESP	2019 - cota FAPESP
Marcello R. B. Andreeta		
Rafael Bonacin de Oliveira	Sem bolsa	2019-2020

IC, MSc, PhD students and post-docs that graduated in July 2020 -2021 / current work			
Edgar Dutra Zanotto			
Ricardo F. Lancelotti/ MSc	MSc	2021	*PhD student*
José Herculis Dantas de Araújo (TCC)	TCC	2018-2020	industry
Mayara Cerruti	IC	2018-2020	student
Anelise Sampaio	TCC	2017-2020	Industry
Marcelo Nalin			

Lia Mara Marcondes	Post-doc	2019-2020	
Ana Candida Martins Rodrigues			
Adriana Nieto Muñoz (Colombia)	PhD	2020	
Jairo Felipe Ortiz Mosquera (Colombia)	PhD	2020	

COVID-19 Efforts for 2020-2021-2022

To attend FAPESP call to the scientific community for studying, understanding and perhaps mitigating the Covid-19 pandemic, we are initiating some pilot projects relating to CeRTEV's expertise:

Solid state sensor for monitoring COVID-19 patients

Marcello Andreeta (DEMa-UFSCar/ CeRTEV)

Since the COVID-19 appeared in our society, there has been a great effort worldwide in order to contain or even exterminate the virus. However, there is a possibility that we might need to coexist with SARS-COV-2 for a long time, such as we still live with HIV virus and influenza. In this way, in order to treat the patients with maximum efficiency, there is the need to monitor them in a real-time mode, since the COVID-19 could change the patient's condition very fast to critical. One way to fulfill this need is to provide small and precise sensors to measure the vital signs of organs affected by the COVID-19. One example is the kidney functions, which could be strongly affected by the COVID-19[1–4]. One example of the importance of knowing all possible parameters of the effect of COVID-19 over the patient has been shown by Liu et al.[3], whose authors proved there, although small, the pH value in the urine of Covid-19 patients can be an indication of the evolution of the disease. They have shown that, among other factors, the urine pH values changes were statistically significant ($p=0.004$). During the last year, besides the fact that Covid-19 has slowed down our experimental research efforts, we were able to implement a new facility in the CeRTEV infrastructure, regarding glass laser melting. This technique is based on an aerodynamic levitation system using compressed air. Using this technique, which is the work related to the master degree of Maíra Dombroski Neme, we were successful in developing a new methodology to produce miniaturized solid-state pH sensors (patent pending). We were able to identify changes in standard pH solutions in the range of pH= 2 to 10. With the acquisition of a new electrometer, we will be able to explore the developed methodology to improve/optimize the sensor.

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An alternative biomaterial approach against COVID-19

Oscar Peitl and E.D. Zanotto (DEMa-UFSCar / CeRTEV)
Marina Trevelin (UFSCar) and Juliana Daguano (UFABC) collaborators

Respiratory diseases due to human coronaviruses SARS-CoV-2 are currently one of the main causes of morbidity and mortality worldwide. As there are currently no effective drugs targeting this virus, the development and study of alternative substances or materials for disease control and to avoid the virus spread are crucial activities. Taking into account the relevance of this matter, our CeRTEV team is currently establishing collaborations with several experts from CTI Renato Archer, IPEN, UFABC and a bioactive glass national company. Namely, Dr. Jorge Silva (CTI), Dr. Daniel Perez and Prof. Janaína Dernowsek (IPEN), Prof. Juliana Daguano (UFABC) and Vetra.

Our main objective is to explore how the virus responds when exposed to bioactive glasses and bio glass-ceramics in different concentrations and bioavailability means.

The viral production is intended to be done in three-dimensional lung multicellular spheroids in air- and liquid-interface using Calu-3 cells (American type culture collection ATCC® HTB55™) in DMEM with 4% of fetal bovine serum and 1% glutamine. Cytopathic effects will be monitored daily under an inverted microscope and after nearly complete cell lysis (approximately 96 h), viral supernatant will be used for inoculation on a 96-well plate with 104 cells/mL. Materials extracts and direct contact will be tested. The chosen concentrations will be 12.5, 25 and 50 mg/ml for two different materials: F18 bioactive glass and Biosilicate (a biphasic glass-ceramic material). The extraction will be done using the manual High Pure RNA Isolation Kit (Roche Life Science), following the recommended procedures and the RT-PCR, using the Roche RealTime PCR Ready RNA Virus Master Kit, will be carried out for relative viral quantification. Tests are intended to be done in triplicate.

To test bioactive materials as a possible treatment, based on “false negative” results, we speculate on the concomitant analysis of the inflammatory response, with macrophage addition to the spheroids. Thus, the infection processes will be monitored every 3 days by the measurement of IL-8, IL-1β and TGF-β from the culture medium, for 15 days (maximum time for virus infection). Since this kind of investigation has no precedent, the outcome is unclear, however, we expect that this investigation can provide some evidence for the potential use of bioactive materials on controlling viruses and cell lysis.

Reusable functional glassy materials focused on nCov-19 annihilation

Andrea de Camargo / LEMAF - Laboratory of Spectroscopy of Functional Materials

The new virus nCoV-2019 is a highly infectious pathogen responsible for the Coronavirus disease that has affected the globe in 2020. Brazil currently occupies the 2nd position in the rank of countries with highest contamination and death figures [1]. Surfaces and objects in general are among the possible transmission channels of the virus. In the absence of effective disinfection methods, the virus can survive from 4h (on paper, for instance) up to 9 days, as it has been observed for ceramic surfaces [2]. Though alcohol and other products can be used for disinfection, they are consumed and only offer short-term antimicrobial action. That motivates the development of longer lasting, reusable disinfection methods based, for instance, on glass and glass ceramic materials. To that end, we propose the development of sol gel derived silicate glassy materials functionalized with antiviral agents such as photosensitizing molecules and metallic nanoparticles. The photosensitizers are molecules that can induce chemical change in other molecules through a photochemical process. Their widespread use is in photodynamic therapy (PDT) of cells and microorganisms through the generation of reactive oxygen species (ROS) which, through oxidation of biomolecules such as proteins and lipids are capable of inducing cell death and deactivation of viruses and bacteria [3,4]. The metallic nanoparticles (MNPs) exhibit well-known antimicrobial action and have been used for combating both viruses and bacteria. Some examples include NPs of silver, gold, iron, iron oxide, copper oxide, zinc oxide, etc. Their mechanism of action depends on the type of the NP and can include photocatalysis, toxicity or generation of ROS.

PLAN OF ACTION: i) Synthesize glassy silicate and organo-silica matrices via the sol gel method from various precursors and in different morphologies (films, bulk, spheres, pellets); ii) From structural characterization select the most resistant matrices that can be easily functionalized; iii) Synthesize, characterize and optimize the antiviral agents (MNPs, photosensitizers) that will be grafted to the vitreous matrices; iv) Functionalize the matrices with the antiviral agents and submit the final materials to biological testing in collaboration with colleagues with the available expertise and infrastructure in Brazil and abroad; v) Select the most efficient material for combating coronavirus; vi) Extend the work focusing on the development of prototypes of masks and glasses, for individual protection, with low cost and encompassing coverage.

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Unfortunately, we have not been able to develop this project in due time since the PhD student designated for that purpose gave up 4 months after having started the project with funding from a special fellowship program of CAPES directed to Covid-related researcher through the Post-graduation Program of Materials Science of EESC/USP.

Optical fibers as fast and cheap sensors for COVID

Marcelo Nalin - LaViE - Laboratório de Vidros Especiais

In order to reduce the use of toxic solvents, decrease the analysis time, and minimize costs, the use of biosensors is an effective option that can provide sensitive analytical responses. Biosensors are characterized by biological recognition using the response driven by an antigen, antibody, or enzyme. [1] When antibodies are used, the biosensor is called an immunosensor, presenting high specificity due to the analyte-antibody bond. [2]

Immunosensors can be prepared using different materials. Portable fiber-based immunosensors used for the monitoring of an evanescent wave absorbance signal offer advantages such as low electromagnetic interference, high transmission bandwidth for optical transfer, fast signal acquisition, and low cost. [3] Enhanced signal transmission can be achieved using conductive polymers such as polyaniline (PANI) or polypyrrole for conversion of the biological signal into an electric signal, from which the analyte concentration is obtained. [4, 5] PANI polymers offer excellent chemical stability and simplicity of synthesis using inexpensive monomers. [6]

U-bent optical fibers have the advantages of robustness, sensitivity, and ease of handling. Furthermore, they can increase sensor sensitivity by up to 10-fold, compared to straight probes. A great advantage of this configuration is increased by the penetration of the evanescent wave field towards the direction of radiation propagation. [7]

The aim of the present project is to develop an ultra-sensitive U-bent optical fiber-based immunosensor for the determination of COVID in blood samples, without any requirement for a sample preparation procedure. The evanescent absorbance can be captured using a low-cost non-hygroscopic silica optical fiber, free from electrical interference and with high signal multiplication capacity, optical transparency, inertness even in aggressive environments, low tendency for laser-induced breakage, and ability to be doped or functionalized by various materials. [8] All these features made this material ideal for use in the present study.

In a recent work (R. Lamarca et al.), Label-free ultrasensitive and environmentally-friendly immunosensor based on a silica optical fiber for determination of ciprofloxacin in wastewater samples, under revision in the journal of Analytical Chemistry (Manuscript ID: ac-2020-02355k)) we demonstrated the versatility of U-bend optical fiber to detect ultra-low concentrations of ciprofloxacin in wastewater samples. We believe that the methodology used in the paper is completely adaptable to develop a cheap sensor to detect COVID virus, however the cooperation with experts in the health field is necessary and is actually under discussion.

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Preparation of amorphous porous thin films functionalized with bismuth species. Detection of and protection from viruses suspended in the atmosphere of crowded indoor gatherings

H. Eckert, IFSC.

Introduction: Increasing evidence has been showing that the suspended aerosol of crowded indoor gatherings constitutes an important vehicle of the severe acute respiratory syndrome Coronavirus (SARS-CoV-2) transmission. Thus, detection of and protection from viral contamination of such aerosols will be an important goal. In pursuit of this objective, we propose to develop a line of research within our CeRTEV effort, dedicated to the development of porous amorphous thin films functionalized with bismuth (III) species. The highly efficient antiviral activity of various bismuth (III) complexes was brought into focus following the last SARS crisis of 2002-2004. [1,2]. Complexes such as bismuth nitrilotriacetate, bismuth nitrate, bismuth tricysteine, and ranitidine bismuth citrate (RBC) turned out to be very efficacious inhibitors of the SARS CoV-2 virus, at micromolar concentration levels. RBC in particular was shown to effectively inhibit the ATPase activities of the helicase and to inhibit the duplex-unwinding activity. [1,2].
Approach: The considerable structural and chemical similarity of SARS- viruses involved in the 2002 and 2019 pandemics [3,4] suggest that Bi complexes may have similar efficacy in the current COVID challenge. The mechanism is thought to involve binding of Bi3+ ions to the cysteine-rich metal binding domain that is located at the N terminus of the SCV helicase protein [1]. If there is indeed an analogous binding interaction (yet to be confirmed) between the new SARS-Cov-2 virus and the bismuth species, the preparation of porous glasses functionalized with bismuth(III) species at their surfaces will offer promising prospects, with regard to both the detection and the removal of the virus from the ambient atmosphere of crowded indoor gatherings.
Virus detection can benefit from the fact that bismuth-doped glasses have a very intense and distinctive luminescence spectrum [5], which can be significantly perturbed by the effect of molecular binding. As a result, one may expect a shift of the emission frequency or possibly altogether suppression (quenching) of the fluorescence, which offers the perspective of developing a solid-state breath analyzer. A second potential application of such a material is the implementation of such porous Bi-doped glasses in antiviral breathing filters.
Work plan: Three different preparation strategies will be explored towards the development of Bi-functionalized amorphous porous surfaces: wet impregnation of

porous siliceous matrices [6], topotactic modification of sol-gel prepared mesoporous sodium aluminosilicate glasses [7] via ion exchange [8] and in-situ templating of porous inorganic frameworks in the presence of the bismuth species [9]. The luminescence characteristics of these materials will be measured and changes in their luminescence spectra upon the binding of thiolic species (such as cysteine) will be characterized. Once the solid materials have been developed and proven their utility in binding studies of model compounds, a collaboration with a virus molecular biology research laboratory will be sought to study the interaction with SARS-Cov-2 virus.

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University-industry involvement through digital events and roadmap in COVID-19 pandemic crisis

Piccirillo, Isabela, Amaral, Daniel Capaldo, Oliveira, Maicon Gouvêa, **Ferreira, Eduardo Bellini**

In the COVID-19 pandemic crisis, the digital collaboration between industries and universities is a necessity for effective solutions development. In this context, the role of virtual involvement becomes essential to interact around a common objective. To support the development of these objectives, technology roadmapping can be a tool to present the directions. An exploratory case study will be selected at glass-making community to involve universities and industries using digital platforms and roadmapping to share knowledge, define common objectives and support partnerships to produce better research results. Through the data comparison from previous face-to-face events and this digital one, it will likely be possible to verify that there was a greater number of participants from different companies and institutions and more collaboration.

Articles on <u>vitreous</u> materials in the period July 2020 – May 2021

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