UNIVERSIDADE FEDERAL DE SÃO CARLOS

PRÓ – REITORIA DE PÓS-GRADUAÇÃO E PESQUISA

FICHA DE CARACTERIZAÇÃO DE DISCIPLINAS

1. Programa de Pós-Graduação em Ciência e Engenharia de Materiais

Início da Validade	Ano	S
	2024	1

2. Objetivo da Ficha Criar disciplina

Código da Disciplina	PPG	Número
	CEM	726

Total de Créditos	05

Nome da Disciplina	Tópicos Especiais em Cerâmicas: Structure, Dynamics and Properties of Vitreous Materials

Campos a Serem Alterados				
Código da Disciplina	Código Anterior	☐ Nome da Disciplina	☐ Carga Horária	
		☐ Créditos	☐ Requisitos	☐ Ementa

Objetivo : Present and discuss the state of the art based on modern, selected, articles on the structure, dynamic processes (diffusion, relaxation and crystallization) and optical, biochemical, electrical and mechanical properties of glassy materials. To present modern computer simulation techniques by molecular dynamics, ab-initio, and artificial intelligence.

3. Carga Horária da Disciplina

3.1. Aulas Teóricas	30	3.2. Aulas Práticas	30	3.3. Exercícios Seminários	15

4. Ementa da Disciplina

	ASSUNTOS
1)	Introduction to the vitreous state
2)	Glass structure by NMR spectroscopy, EPR and Raman Scattering
3)	Relaxation, sintering and crystallization of glasses
4)	Design and properties of glass-ceramics (GCs)
5)	Optical properties of glasses and GCs
6)	Electrical properties of glasses and GCs
7)	Biochemical properties of glasses and GCs
8)	Mechanical properties of glasses and GCs
9)	Simulation of glass structure and properties by molecular dynamics
10)	Simulation of glass structure and properties by ab-initio methods
11)	Machine learning approach for novel glass design

5. Caráter da Disciplina

☐ Obrigatória para: ☐ Doutorado ☐ Mestrado ☐ Ambos

☐ Especifica da Área de Concentração em :

☒ Optativa para: ☐ Doutorado ☐ Mestrado ☒ Ambos

6. Disciplinas Pré – Requisitos, se houver

Código	Nome
1-	

7. Bibliografia Principal

(autor, Título, ano da Publicação e Editora)

1)	**Introduction to the glassy state of matter**
1.1)	**Zanotto, E.D.,** Mauro, J.C. The **glassy state** of matter: Its definition and ultimate fate (2017) Journal of Non-Crystalline Solids, 471, pp. 490-495
1.2)	Welch, R.S., **Zanotto, E.D.,** Wilkinson, C.J., Cassar, D.R., Montazerian, M., Mauro, J.C. Cracking the **Kauzmann paradox** (2023) Acta Materialia, 254, art. no. 118994
2)	**NMR and EPR spectroscopies**
2.1)	Ardelean I., Cora S., Rusu D. Ardelean, I. Cora, Simona, Rusu, Dorina **EPR** and FT-IR spectroscopic studies of Bi2O3-B2O3-CuO glasses (2008) Physica B: Condensed Matter, 403 (19-20), pp. 3682 - 3685,
2.2)	**De Oliveira M.,** Uesbeck T., Gonçalves T.S., Magon C.J., **Pizani P.S., De Camargo A.S.S., Eckert H.** Network Structure and Rare-Earth Ion Local Environments in Fluoride Phosphate Photonic Glasses Studied by Solid-State NMR and Electron Paramagnetic Resonance Spectroscopies (2015) Journal of Physical Chemistry C, 119 (43), pp. 24574 - 24587,
2.3)	**Eckert, H.** Structural characterization of noncrystalline solids and glasses using solid state **NMR** (1992) Progress in Nuclear Magnetic Resonance Spectroscopy, 24 (3), pp. 159-293.
2.4)	Mohammadi, H., Mendes Da Silva, R., Zeidler, A., Gammond, L.V.D., Gehlhaar, F., **De Oliveira, M.**, Jr., Damasceno, H., **Eckert, H.,** Youngman, R.E., Aitken, B.G., Fischer, H.E., Kohlmann, H., Cormier, L., Benmore, C.J., Salmon, P.S. Structure of diopside, enstatite, and magnesium aluminosilicate glasses: A joint approach using neutron and x-ray diffraction and solid-state **NMR** (2022) Journal of Chemical Physics, 157 (21), art. no. 214503,
2.5)	**de Oliveira, M.,** Jr., Damasceno, H., Salmon, P.S., **Eckert, H.** Analysis and information content of quadrupolar NMR in glasses: 25Mg **NMR** in vitreous MgSiO3 and CaMgSi2O6 (2022) Journal of Magnetic Resonance Open, 12-13, art. no. 100067,
3)	**Raman spectroscopy**
3.1)	Moulton, B.J.A., Silva, L.D., Doerenkamp, C., Lozano, H., **Zanotto, E.D., Eckert, H., Pizani, P.S.** Speciation and polymerization in a barium silicate glass: Evidence from 29Si NMR and **Raman** spectroscopies (2021) Chemical Geology, 586, art. no. 120611,
3.2)	Pena, R.B., Sampaio, D.V., Lancelotti, R.F., Cunha, T.R., **Zanotto, E.D., Pizani, P.S.** In-situ **Raman spectroscopy** unveils metastable crystallization in lead metasilicate glass (2020) Journal of Non-Crystalline Solids, 546, art. no. 120254,
4)	**Glass crystallization**
4.1)	**Zanotto, E.D.,** Tsuchida, J.E., Schneider, J.F., **Eckert, H.** Thirty-year quest for **structure-nucleation** relationships in oxide glasses (2015) International Materials Reviews, 60 (7), pp. 376-391
4.2)	Montazerian, M., **Zanotto, E.D.** Nucleation, Growth, and **Crystallization** in Oxide Glass-formers. A Current Perspective (2022) Reviews in Mineralogy and Geochemistry, 87, pp. 405-429
4.3)	Fokin, V.M., **Zanotto, E.D.,** Yuritsyn, N.S., Schmelzer, J.W.P. Homogeneous **crystal nucleation** in silicate glasses: A 40 years perspective (2006) Journal of Non-Crystalline Solids, 352 (26-27), pp. 2681-2714.

5)	**Sintering of glasses and glass-ceramics**
5.1)	Prado, M.O., Nascimento, M.L.F., **Zanotto, E.D.** On the **sinterability** of crystallizing glass powders (2008) Journal of Non-Crystalline Solids, 354 (40-41), pp. 4589-4597
5.2)	Blaeß, C., **Müller, R.,** Poologasundarampillai, G., Brauer, D.S. **Sintering** and concomitant crystallization of bioactive glasses (2019) International Journal of Applied Glass Science, 10 (4), pp. 449-462.
5.3)	Oscar Prado, M., **Dutra Zanotto, E., Müller, R.** Model for **sintering** polydispersed glass particles (2001) Journal of Non-Crystalline Solids, 279 (2-3), pp. 169-178.
6)	**Glass-ceramics**
6.1)	Campos, J.V., Lavagnini, I.R., Zallocco, V.M., **Ferreira, E.B.,** Pallone, E.M.J.A., Rodrigues, A.C.M. Flash **sintering with concurrent crystallization** of Li1.5Al0.5Ge1.5(PO4)3 glass (2023) Acta Materialia, 244, art. no. 118593,
6.2)	Fernandes, R.G., Reis, R.M.C.V., Tobar, R.R., **Zanotto, E.D**., **Ferreira, E.B.** Simulation and experimental study of the particle size distribution and pore effect on the **crystallization of glass powders** (2019) Acta Materialia, 175, pp. 130-139.
6.3)	**Ferreira, E.B., Zanotto, E.D.,** Scudeller, L.A.M. Glass and **glass-ceramic** from basic oxygen furnace (BOF) slag (2002) Glass Science and Technology: Glastechnische Berichte, 75 (2), pp. 75-86
6.4)	**Zanotto, E.D.** A bright future for **glass-ceramics** (2010) American Ceramic Society Bulletin, 89 (8), pp. 19-27.
7)	**Electrical properties of glass**
7.1)	Nieto-Muñoz, A.M., Ortiz-Mosquera, J.F., **Rodrigues, A.C.M.** The impact of heat-treatment protocol on the grain size and **ionic conductivity** of NASICON glass-ceramics (2020) Journal of the European Ceramic Society, 40 (15), pp. 5634-5645. Cited
7.2)	d'Anciães Almeida Silva, I., Nieto-Muñoz, A.M., **Rodrigues, A.C.M., Eckert, H.** Structure and **lithium-ion mobility** in Li1.5M0.5Ge1.5(PO4)3 (M = Ga, Sc, Y) NASICON glass-ceramics (2020) Journal of the American Ceramic Society, 103 (7), pp. 4002-4012.
8)	**Bio properties**
8.1)	**Peitl, O., Dutra Zanotto, E**., Hench, L.L. Highly **bioactive** P2O5-Na2O-CaO-SiO2 glass-ceramics (2001) Journal of Non-Crystalline Solids, 292 (1-3), pp. 115-126.
8.2)	Crovace, M.C., Souza, M.T., Chinaglia, C.R., **Peitl, O., Zanotto, E.D.** Biosilicate® - A multipurpose, highly **bioactive** glass-ceramic. In vitro, in vivo and clinical trials (2016) Journal of Non-Crystalline Solids, 432, pp. 90-110.
9)	**Mechanical properties**
9.1)	**Serbena, F.C.,** Mathias, I., Foerster, C.E., **Zanotto, E.D.** Crystallization **toughening** of a model glass-ceramic (2015) Acta Materialia, 86, pp. 216-228.
9.2)	Senk, M.V., Mathias, I., **Zanotto, E.D., Serbena, F.C.** Crystallized fraction and crystal size effects on the **strength and toughness** of lithium disilicate glass-ceramics (2023) Journal of the European Ceramic Society, 43 (8), pp. 3600-3609
10)	**Optical Properties and photonic glasses**
10.1)	Herrera, A., Fernandes, R.G., **De Camargo, A.S.S**., Hernandes, A.C., Buchner, S., Jacinto, C., Balzaretti, N.M. **Visible-NIR emission** and structural properties of Sm3+ doped heavy-metal oxide glass with composition B2O3-PbO-Bi2O3-GeO2 (2016) Journal of Luminescence, 171, pp. 106-111.
10.2)	Dousti, M.R., Poirier, G.Y., **De Camargo, A.S.S.** Structural and **spectroscopic characteristics** of Eu3+-doped tungsten phosphate glasses (2015) Optical Materials, 45, pp. 185-190.
10.3)	Rajesh, D., Amjad, R.J., Reza Dousti, M., **de Camargo, A.S.S.** Enhanced **VIS and NIR emissions** of Pr3+ions in TZYN glasses containing silver ions and nanoparticles (2017) Journal of Alloys and Compounds, 695, pp. 607-612.
10.4)	Blanc, W., Gyu Choi, Y., Zhang, X., **Nalin, M.,** Richardson, K.A., Righini, G.C., Ferrari, M., Jha, A., Massera, J., Jiang, S., Ballato, J., Petit, L. The past, present and future of **photonic glasses**: A review in homage to the United Nations International Year of glass 2022 (2023) Progress in Materials Science, 134, art. no. 101084,
10.5)	Marcondes, L.M., Silva, M.C.D.C., Franco, D.F., Manzani, D., Poirier, G.Y., **Nalin, M.** Monitoring Ag nanoparticles growth in undoped and Er3+ doped glasses by in-situ UV–Vis spectroscopy and its **luminescent properties** (2023) Journal of Non-Crystalline Solids, 609, art. no. 122286,

11)	**Molecular dynamics simulations**
11.1)	Separdar, L., **Rino, J.P., Zanotto, E.D.** **Molecular dynamics simulations** of spontaneous and seeded nucleation and theoretical calculations for zinc selenide (2021) Computational Materials Science, 187, art. no. 110124,
11.2)	Tipeev, A.O., **Zanotto, E.D., Rino, J.P.** Crystal Nucleation Kinetics in Supercooled Germanium: **MD Simulations** versus Experimental Data (2020) Journal of Physical Chemistry B, 124 (36), pp. 7979-7988.
12)	**Ab-initio simulations**
12.1)	Yadav, A., Acosta, C.M., **Dalpian, G.M.,** Malyi, O.I. **First-principles** investigations of 2D materials: Challenges and best practices (2023) Matter, 6 (9), pp. 2711-2734.
12.2)	Schleder, G.R., Padilha, A.C.M., Reily Rocha, A., **Dalpian, G.M.,** Fazzio, A. **Ab Initio** Simulations and Materials Chemistry in the Age of Big Data (2020) Journal of Chemical Information and Modeling, 60 (2), pp. 452-459.
13)	**Machine Learning approaches**
13.1)	Mastelini, S.M., **Cassar, D.R.,** Alcobaça, E., Botari, T., de Carvalho, A.C.P.L.F., **Zanotto, E.D.** **Machine learning** unveils composition-property relationships in chalcogenide glasses (2022) Acta Materialia, 240, art. no. 118302,
13.2)	**Cassar, D.R.,** Santos, G.G., Zanotto, E.D. Designing optical glasses by **machine learning** coupled with a genetic algorithm (2021) Ceramics International, 47 (8), pp. 10555-10564

8. Principais Docentes Responsáveis

Vínculo

1) Prof. Dr. Edgar Dutra Zanotto ☒

9. Aprovação da Coordenação do Programa de Pós-Graduação

Esta Ficha de Caracterização foi aprovada na 664ª reunião da CPG-PPGCEM de 10/10/2023 deste Programa de Pós-Graduação.

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18 / 10 / 2023

Assinatura do Coordenador do Programa

10. Aprovação pelo Conselho Interdepartamental do Centro de Ciências Exatas e de Tecnologia - CCET

Aprovada na ______.ª Reunião da CAEPE/CCET, realizada em _____ / _____ / ________.

Assinatura do Diretor do Centro

11. Aprovação da Câmara de Pós-Graduação e Pesquisa

Aprovada na _______.ª Reunião da Câmara de Pós-Graduação e Pesquisa, realizada em _____/_____/______.

Assinatura do Presidente da Câmara