



UNIVERSIDADE FEDERAL DE SÃO CARLOS - UFSCar
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DEPARTAMENTO DE ENGENHARIA DE MATERIAIS – DEMa
PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIA E ENG. DE MATERIAIS - PPGCEM



INTERNATIONAL SEMINARS IN MATERIALS SCIENCE AND ENGINEERING OF DEMa/PPGCEM-UFSCar

PRESSURE AND COMPOSITION EFFECTS ON GLASS STRUCTURE AND GLASS TRANSITION: INSIGHTS FROM ATOMISTIC COMPUTER SIMULATIONS

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Abstract:

The structure of glass depends on the composition, as well the thermal and pressure history. The structural variations in turn impact the glass relaxation, transition, crystallization behaviors and the properties. Various experimental techniques have been used to characterize the structure and behaviors of glasses but, due to complexity of structure and amorphous nature, glass structure poses as a significant challenge to existing experimental approaches. Atomistic computer simulations, on the other hand, have been developed and their applications fast progressing to complement experimental methods to understand glass structures and behaviors. In this talk, I will provide an overview of the field then use a few examples to illustrate the applications of molecular dynamics simulations in the understanding pressure and composition effect on glass structure and behaviors as a result from my visit to the CeRTEV of UFSCar as a Fulbright US Scholar early in 2020. Results of ongoing projects to investigate the pressure effect on the glass formation and glass transition in MgO-Al₂O₃-SiO₂ glasses, structural change (particularly the formation of five-fold coordinated silicon) as a function of composition in phosphosilicate glasses, and cooling rate effect on the structures of lithium disilicate glasses. The progresses on these mini-projects signify of the importance of collaborations between experimental and simulation efforts on glass research, as well as the importance of international interactions and cultural exchanges on advancing scientific fields including advanced materials researches.

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Time: 4 pm (São Carlos time)

Location: link <https://meet.google.com/hie-dcyp-bxo>