UFRPE - UACSA

Campus das Engenharias

COLÓQUIOS DA PÓS-GRADUAÇÃO EM ENGENHARIA FÍSICA

" Relaxation, crystal nucleation and Kauzmann temperature in supercooled zinc selenide"

The liquid to crystal transition is a ubiquitous phenomenon, which is a very important scientific and technological subject in diverse fields, such as biology, mineral formation, semiconducting materials, water and metal solidification, glass-ceramics and glass formation. Due to its substantial scientific and technological relevance, understanding and describing the **relaxation**, **crystallization mechanisms** and **kinetics** of liquids during cooling process is relevant, fascinating and challenging. Structural relaxation is a key phenomenon that plays a significant role on vitrification and crystallization. If a liquid is deeply supercooled without vitrifying or crystallizing, a particularly intriguing possibility is that it could reach the isentropic temperature, T_K, predicted by Kauzmann, at which the difference between the entropy of the supercooled liquid (SCL) and its isochemical crystal (excess entropy) vanishes, known as the **Kauzmann paradox. The main question is: what is the ultimate fate of supercooling?** ***If the ultimate fate of cooling a supercooled be crystallization how this crystallization occurs?*** In this talk, first I will provide an overview of the field and the most well-known theory in this field, the Classical Nucleation Theory. Then I will present the results obtained from molecular dynamics simulation, with focusing on thermodynamic and kinetic properties such as the Kauzmann temperature, T_K (where the excess entropy tends to zero), the kinetic spinodal temperature, T_{ks} (where the relaxation and crystal nucleation curves cross), the glass transition temperature, T_g spontaneous and seeded nucleation and theoretical calculations based on the Classical Nucleation Theory in model system **zinc selenide.**

Leila Separdar

Department of Physics, Federal University of São Carlos

Dia: 12/04/2021 (Segunda-feira) **Horário: 16:00 h**

Transmissão: Aplicativo meet (link: https://meet.google.com/pog-tdji-xqp)