Instituto de Física UFRJ

INSTITUTO DE QUÍMICA
Universidade Federal do Rio de Janeiro

Interdisciplinary Workshop
on Theoretical and Computational Techniques for Material Science

Special guest: **Prof. Dr. Stephen C. Parker**
University of Bath, UK

Prof. Dr. Stephen C. Parker is a well-known expert in surface science, developing and applying computational techniques to model defects, the thermodynamics and phase transitions in minerals and studying oxides properties. He is the author of the code **METADISE** to simulate surfaces and interfaces of solids using classical methods.

Aim of the workshop: An introduction on theoretical techniques will be done for inexpert modellers from different scientific backgrounds (mainly physicists and chemists). It will be related to key fields of research on ***nanotechnology, inorganic chemistry, engineering, solid materials, catalysis and energy materials***. In the first part, lectures and tutorials will be given by C. Arrouvel and S. C. Parker in order to 1/ access to the new functionalities in METADISE code, 2/ introduce classical Molecular Dynamics. The second part is dedicated to electronic structures with advanced lectures/tutorials given by local professors.

Max of participants : 50 ; if possible, bring a laptop (Windows).

Dr. Corinne Arrouvel
Coordenador
IQ – UFRJ/UFSCar
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Local: IQ, CT, UFRJ – sala A601

Date: **21-23 of March 2018**

Duration: 15h [9h-12h ; 14h-17h]

21st of March, Corinne Arrouvel / **Stephen C. Parker**
Molecular Mechanics and Molecular Dynamics (6h)

22nd of March, Rodrigo Capaz / Marcos Menezes (IF-UFRJ)
DFT and 2D Materials (3h)
Luciano Costa (UFF)
Molecular Dynamics and QM/MM (3h)

23rd of March, Daniel Reyes (IME)
Superconductors and Quasicrystals (1h)
Ricardo Rodrigues (IQ-UFRJ)
DFT and 3D Materials/Surfaces (1h30)
Round Table (30mn)

Social meeting: 22nd of March, Boteco