United Nations Educational, Scientific and Cultural Organization

ICTP - East African Institute for Fundamental Research under the auspices of UNESCO

DEFECTS in CRYSTALS

18 November – 22 November, 2019

University of Rwanda, Kigali, Rwanda

Background and purpose

By intentionally creating defects in materials, we can tune/change their properties. For example, by adding zinc to copper ("alloying"), we create brass which is stronger and harder than copper; ruby and sapphire are both aluminum oxide but look very different because they contain different impurity defects. Understanding defects can help us in creating novel useful materials. An intense 5-day school will be conducted at the ICTP-EAIFR premises of the University of Rwanda, Kigali in order to introduce participants to defects in crystals. The school will consist of morning lectures and problems, combined with afternoon hands-on sessions to calculate defect properties using standard freely available codes. The students will learn to understand the route from quantities that can be calculated at the atomic scale, using variants of Kohn-Sham density functional theory or interatomic potentials, to measurable thermodynamic properties.

Instructors:

□ Prof. Michael Finnis (Imperial College)

□ Dr. Thomas Mellan (Imperial College)

Topics to be covered:

1) Thermodynamics of Interfaces
   - Definition of interface (or surface) free energy
   - Interface excess quantities and the Gibbs adsorption equation (1,2 and more components; 1 or 2 phases).
   - The gamma surface and the Wulff and Winterbottom constructions for crystal and precipitate morphology
2) Atomistic structure of interfaces and computation of properties
   - Coincident site lattice, "Displacement Shift Complete" (DSC) lattice, periodic boundary conditions.
   - The distinction between surface energy and surface tension (or surface stress)
   - Effect of lattice vibrations
3) Point defects
   - Formation energies and concentrations of vacancies in elements and ordered compounds (theory and computation).
   - Effect on phase diagrams - Case studies: NiAl and ZrC - Segregation to interfaces

Participation Information

University lecturers in solid state physics, solid state chemistry, materials science and related fields, as well as advanced post-graduate students (masters and doctoral levels) are encouraged to apply. Women candidates are strongly encouraged to apply. Selection of participants will be based on their technical background. Priority will be given to applicants who will be presenting posters of their current work. There is no registration fee. A limited number of grants are available to support attendance of some selected participants. To apply, send your CV to: **workshop20191118@eaifr.org and fill the form here:** https://forms.gle/bRqugaQngpcfPxz99

Deadline for application: October 22, 2019

For further information contact: info@eaifr.org or workshop20191118@eaifr.org