Interface properties from atomistic simulations

We are seeking postdoctoral researchers and graduate students who are interested in developing and applying new hybrid computational approaches to study the interaction of solute atoms with solid/solid interfaces. The project builds on previous work at UBC that provides insight into the physics of solute diffusion due to the presence of atomistic, crystalline defects and the resulting structural changes in the material. On the ab-initio level, we plan to further improve and apply a QM/MM scheme [1] that couples a small region treated by density functional theory with a much larger boundary region described by classical force fields. These calculations provide access to binding energies and diffusivities with high chemical accuracy, but are restricted to static (zero temperature) situations. In order to study dynamical phenomena such as defect induced precipitation or phase separation, we plan to employ a dynamical classical density functional approach that treats the atomistic topology of a crystalline material by density fields and evolves the alloy composition based on an approximated atomistic free energy functional and continuum description of mass transport [2,3]. As a result, we can study diffusion processes that are inaccessible with particle based molecular dynamics simulations but retain crucial aspects of the discrete nature of matter.

The ideal candidate for this position will have a background in condensed matter physics and/or materials science/engineering with experience with atomistic simulation (DFT, molecular dynamics, Monte Carlo, classical density functional theory) and good computational skills (e.g. C++, python).

References:

[1] L. Huber et al., Computational Materials Science 118, 259 (2016)
[2] E. Dontsova, J. Rottler, and C. W. Sinclair, Phys. Rev. B 90, 174102 (2014)
[3] E. Dontsova, J. Rottler, and C. W. Sinclair, Phys. Rev. B 91, 224103 (2015)

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