MM 24: HV Finnis

Time: Wednesday 14:00–14:30 Location: IFW A

Invited Talk MM 24.1 Wed 14:00 IFW A

Statistical thermodynamics of defects and interfaces in metals

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In order to make more impact in metal physics, and especially engineering, theorists working at the atomic scale are turning increasing attention to understanding and predicting high temperature properties. One of the challenges this entails is the application of statistical mechanical techniques, via computer simulation, using models based on electron theory for calculating internal energies. In this talk I will briefly review how techniques for free energy calculation (classical density functional theory, atomistic thermodynamics, biased molecular dynamics sampling, such as metadynamics and Wang-Landau methods) are being linked to techniques for internal energy calculation, with examples of our work including point defect concentrations, melting temperature and solid-liquid interfacial free energies in general. The emphasis is on how we can go beyond regular solution theory and the quasi-harmonic approximation. 1. Hagen, M. et al, Point defects and chemical potentials in ordered alloys. Phil. Mag. A 1998, 77, 447-464. 2. Angioletti-Uberti, S. et al, Solid-Liquid Interface Free Energy through Metadynamics Simulations. Phys. Rev. B 2010, 81, 125416.