ICAMS Special Seminar

Wednesday, 07 March, 11:00 a.m.
Room IC 02-718

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Tight binding theory of interstitials in metals

I will recall our approach to the polarisable ion and magnetic tight binding approximation, including its application to organic molecules and water; and then focus on the transition metals and their interstitial elements, oxygen, carbon and hydrogen. I will demonstrate tight binding molecular dynamics and statics to study carbon and hydrogen diffusivity and binding to vacancies in ferrite. I will outline future plans for how to calculate interstitial binding to dislocations with a view to upscaling to kinetic Monte Carlo and discrete dislocation dynamics, leading to possible interpretations of observed effects of interstitials on the behaviour of individual dislocations. I will also discuss how we approach the problem of quantum fluctuations of the proton and how we will pursue this in future work.