Warwick Centre for Predictive Modelling Seminar Series

Predictive Modelling: a view from the atomic level

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R0.12, Ramphal Building, Ground Floor

Abstract: One of the more powerful aspects of molecular modelling is the ability it gives to identify and characterise novel and unexpected mechanisms that affect the properties of complex materials. In this talk I will summarise some of the work that has been done within my group with adaptive molecular dynamics and global optimisation methods, and will give examples of the mechanistic insight this has yielded in applications to nanoparticle formation, crystal nucleation, and biomolecular function. In the process I will discuss some of the issues for data dimensionality reduction and characterising free energy hypersurfaces that arise with these applications.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars