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Predictive Multi-scale Modelling: an Interdisciplinary Perspective and the Case of Density Embedding Methods

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D202 Seminar room, School of Engineering, 2nd Floor

Abstract: Multi-scale modelling has become increasingly important in many scientific areas and industrial applications. The vision of simulating a whole air plane or the toxicity of a new drug in a human cell requires to consistently and reliably simulate a huge variety of physical and chemical effects while at the same time coupling across a multiplicity of lengths and time scales.
In the first part of my talk I will give you an overview about current state-of-the-art multi-scale modelling techniques, touching on persistent challenges as well as open questions. In the second part of my talk I will present you insights about the quality of the embedded atom methods (EAM).
In this presentation I will address the following questions:

- Where can these models break down, for example the EAM (Truhlar & coworkers) and the modified EAM (Baskes & coworkers) for CH4 on Ni(100)?
- How can existing models be improved?
- How can we choose a good model?

Ultimately, modelling of drugs and materials will be moved to a level where a careful reliability check of the simulations goes hand in hand with the design of new optimised medications, catalysts and functional materials.

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

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