INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Monday, January 9, 4:30 p.m. ICAMS Seminar room UHW 11/1102

Exploring Energy Landscapes: From Molecules to Nanodevices

Coarse-graining the potential energy surface into the basins of attraction of local minima provides a computational framework for investigating structure, dynamics and thermodynamics in molecular science. Steps between local minima form the basis for global optimisation via basin-hopping and for calculating thermodynamic properties using the superposition approach and basin-sampling. To treat global dynamics we must include transition states of the potential energy surface, which link local minima via steepest-descent paths. We may then apply the discrete path sampling method, which provides access to rate constants for rare events. In large systems the paths between minima with unrelated structures may involve hundreds of stationary points of the potential energy surface.
New algorithms have been developed for both geometry optimisation and finding connections between distant local minima, which allow us to treat such systems. A graph transformation approach enables rate constants and committor probabilities to be extracted from kinetic transition networks containing over a million states. Applications will be presented for a range of different examples, including atomic and molecular clusters, biomolecules, condensed matter, and coarse-grained models of mesoscopic structures.

Selected Publications:

D.J. Wales, Curr. Op. Struct. Biol., 20, 3-10 (2010)
D.J. Wales, J. Chem. Phys., 130, 204111 (2009)
B. Strodel and D.J. Wales, Chem. Phys. Lett., 466, 105-115 (2008)
D.J. Wales and T.V. Bogdan, J. Phys. Chem. B, 110, 20765-20776 (2006)
D.J. Wales, Int. Rev. Phys. Chem., 25, 237-282 (2006)
D.J. Wales, "Energy Landscapes", Cambridge University Press, Cambridge, 2003