

# Energy landscapes for Self-Assembly

David Wales

## 1. Abstract

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will summarise new approaches for global optimisation, enhanced sampling for systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented focussing on design principles for structures based on shells, including coarse-grained models of mesoscopic systems.

### Selected Publications:

Design of self-assembling mesoscopic Goldberg polyhedra

I Horvath, DJ Wales, SN Fejer – *Nanoscale Adv* (2022) 4, 4272

(doi: 10.1039/d2na00447j)

Emergent Complexity from Simple Anisotropic Building Blocks: Shells, Tubes and Spirals

SN Fejer, D Chakrabarti, DJ Wales – *ACS Nano* (2010) 4, 219

(doi: 10.1021/nn9013565)

*Ann. Rev. Phys. Chem.*, 69, 401-425, (2017). Exploring Energy Landscapes

*Chem. Commun*, 53, 6974-6988 (2017). Exploring biomolecular energy landscapes

Energy Landscapes: Some New Horizons, *Curr. Op. Struct. Biol.*, 20, 3-10, 2010.

Energy Landscapes, Cambridge University Press, Cambridge, 2003