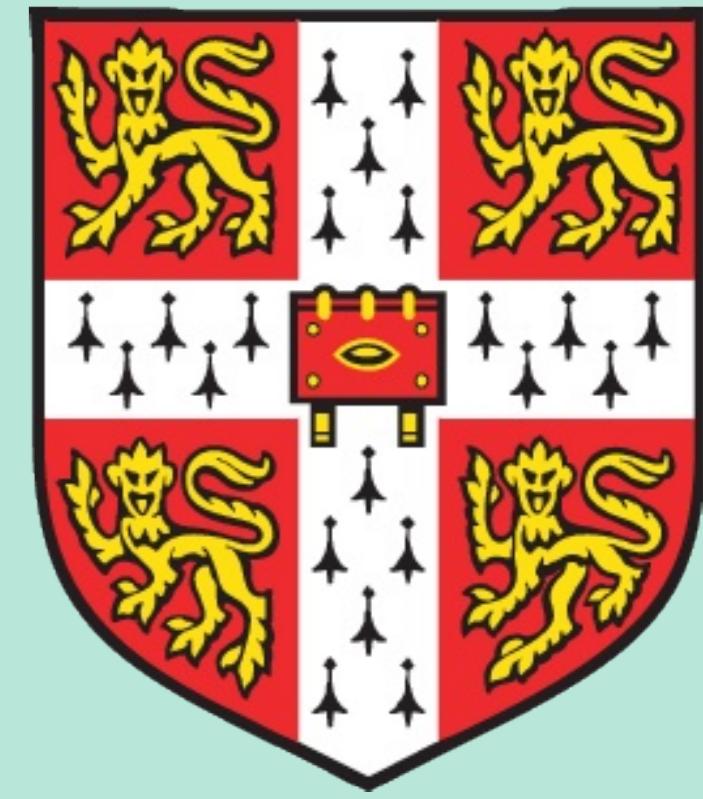


Application of basin-hopping global optimization in the context of energy landscape exploration



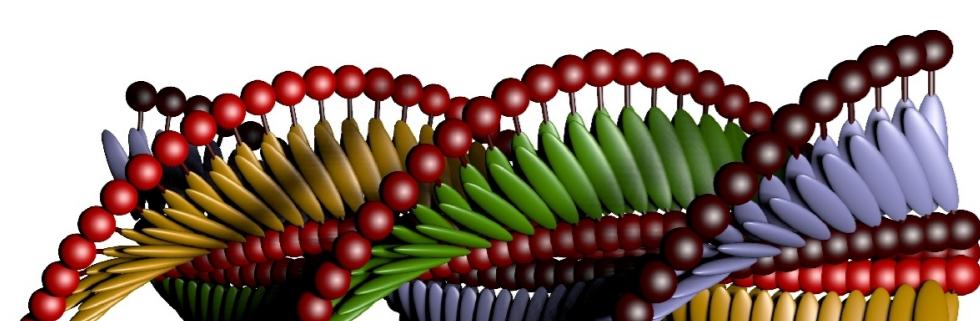
Jacob Stevenson, Victor Rühle, David Wales
*Department of Chemistry, University of Cambridge
 Lensfield Road, Cambridge, CB2 1EW*

Basin-hopping

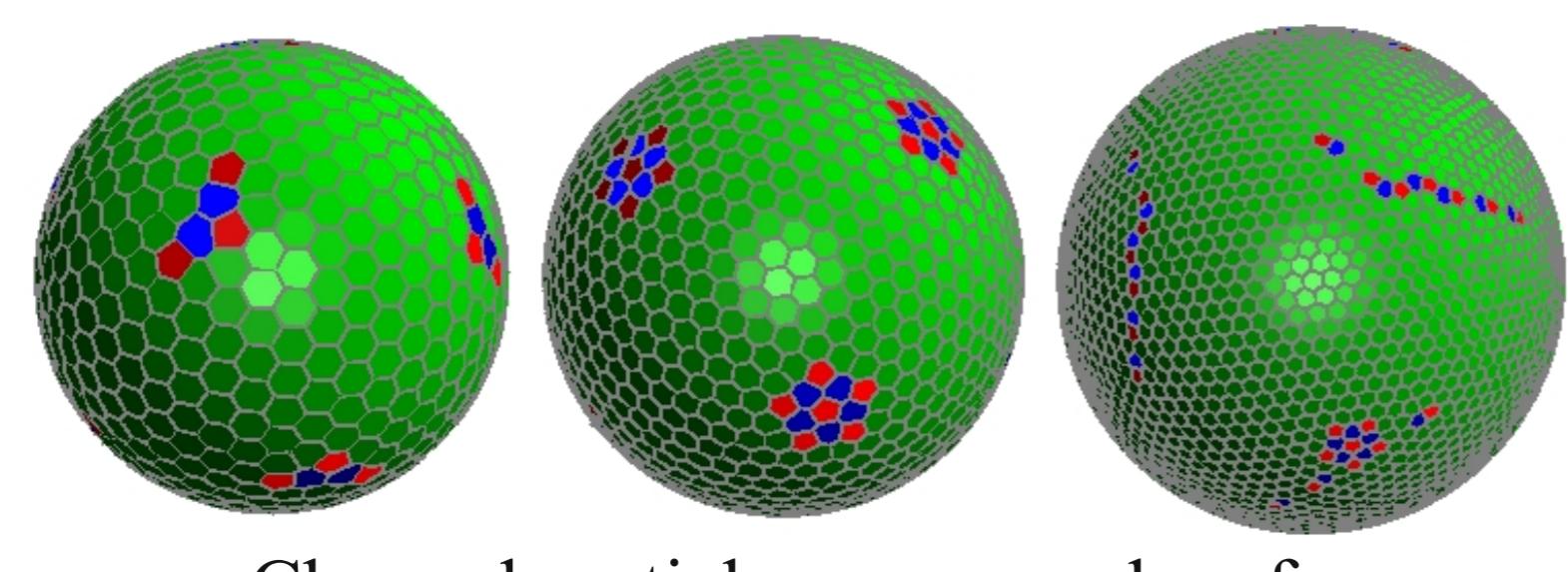
Basin-hopping is a stochastic algorithm for finding the global minimum of a smooth scalar function of one or more variables. It is implemented in SciPy (version 0.12) as

`scipy.optimize.basin hopping`

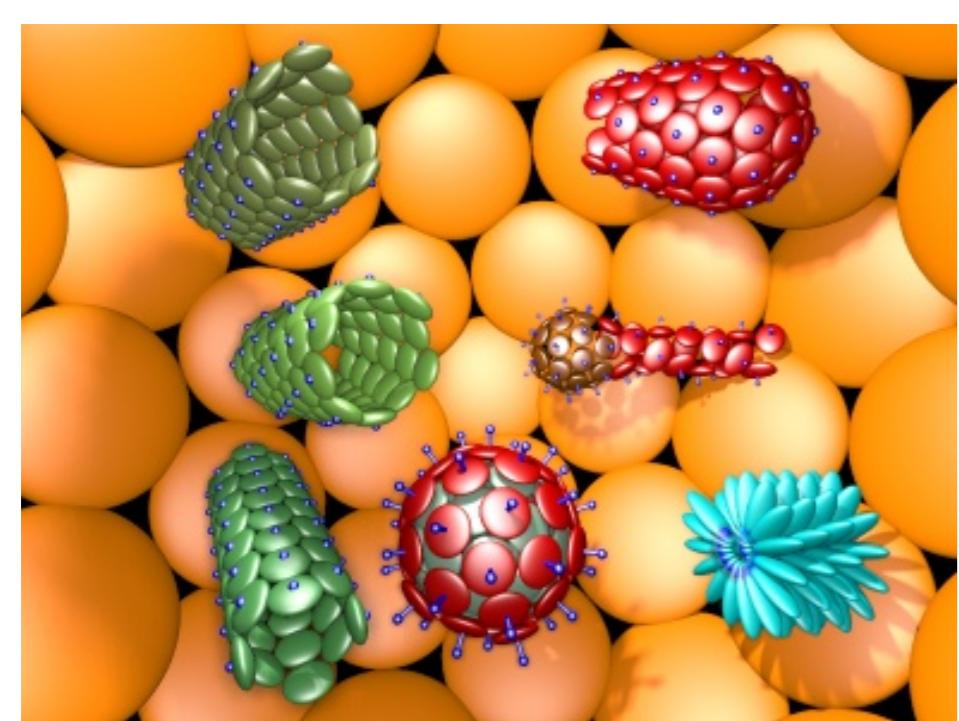
Global optimization is a crucial tool in many areas of physics, chemistry and biology. This is generally framed in terms of finding the molecular or atomic structures that minimize the energy. Some examples of systems that have been studied with basin hopping are:



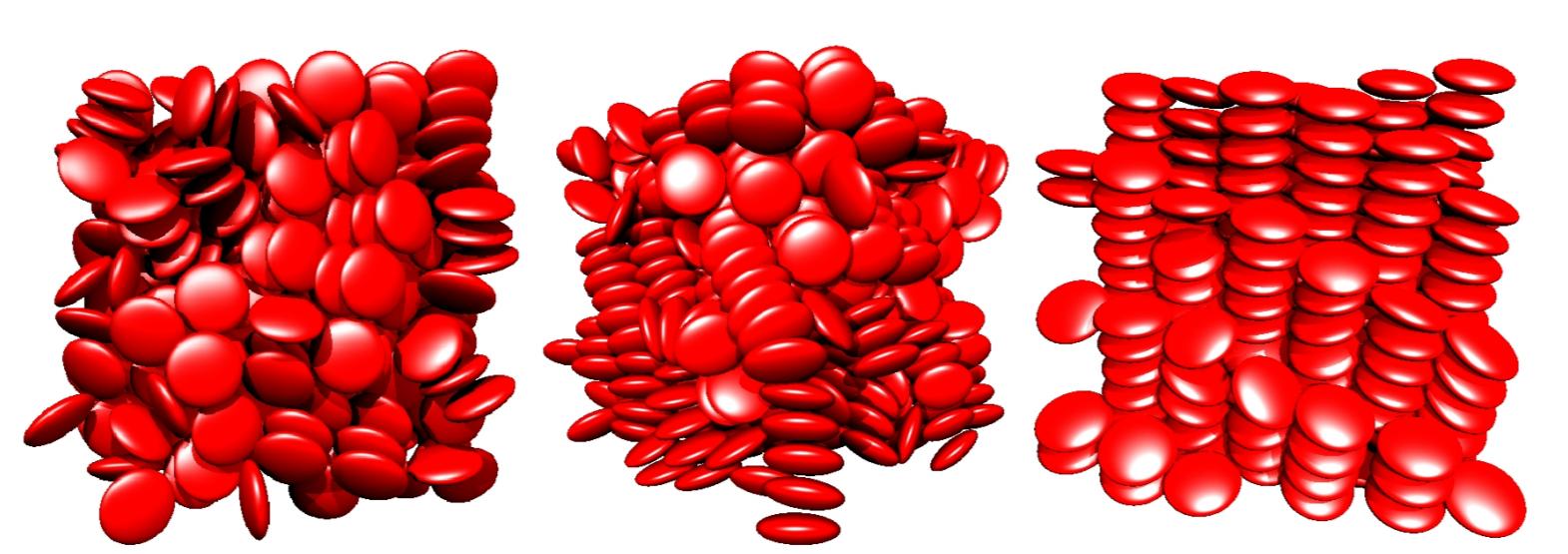
Protein self-assembly



Charged particles on curved surfaces (Thomson problem)



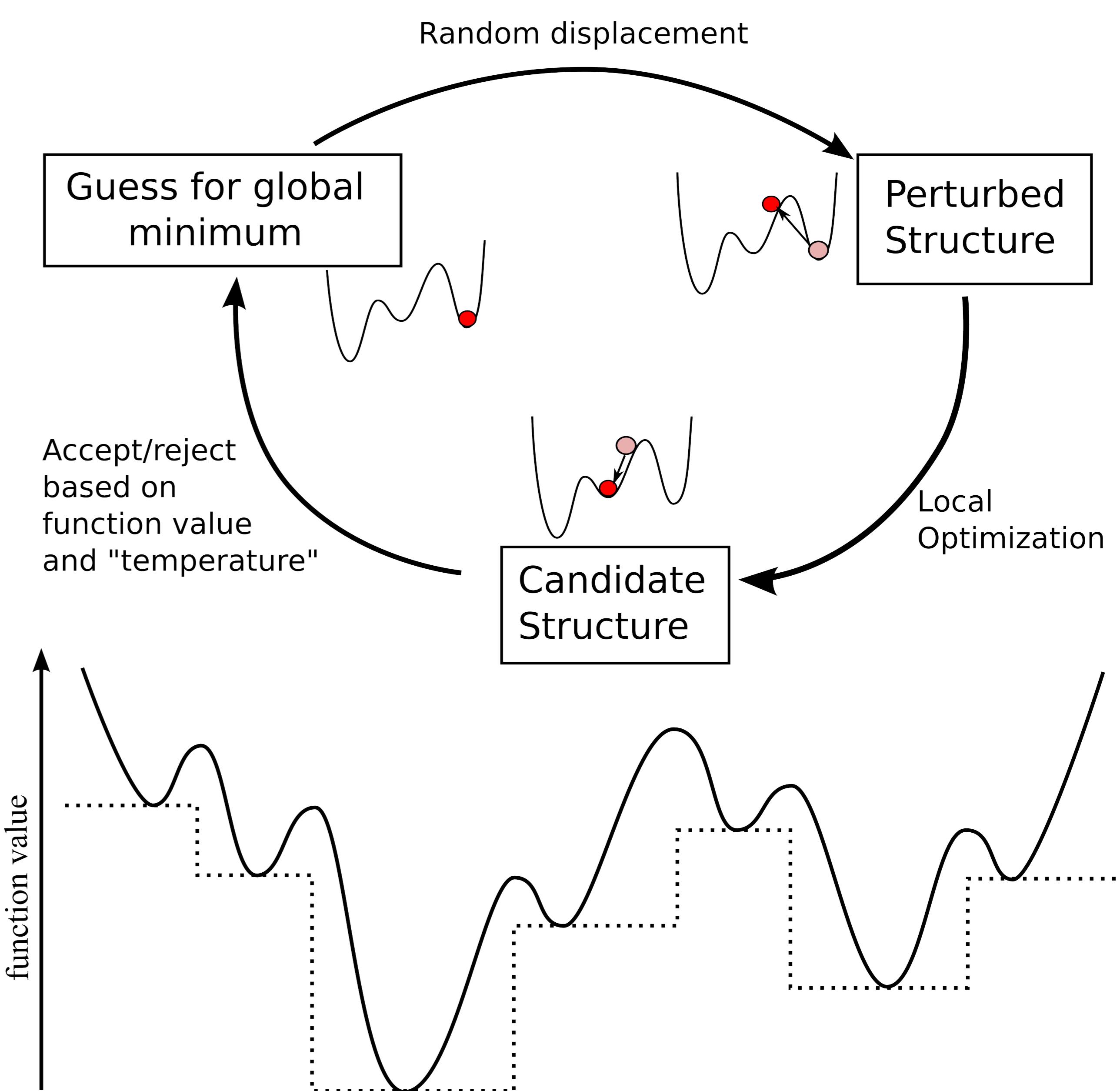
Virus capsid formation



Discotic liquid crystals

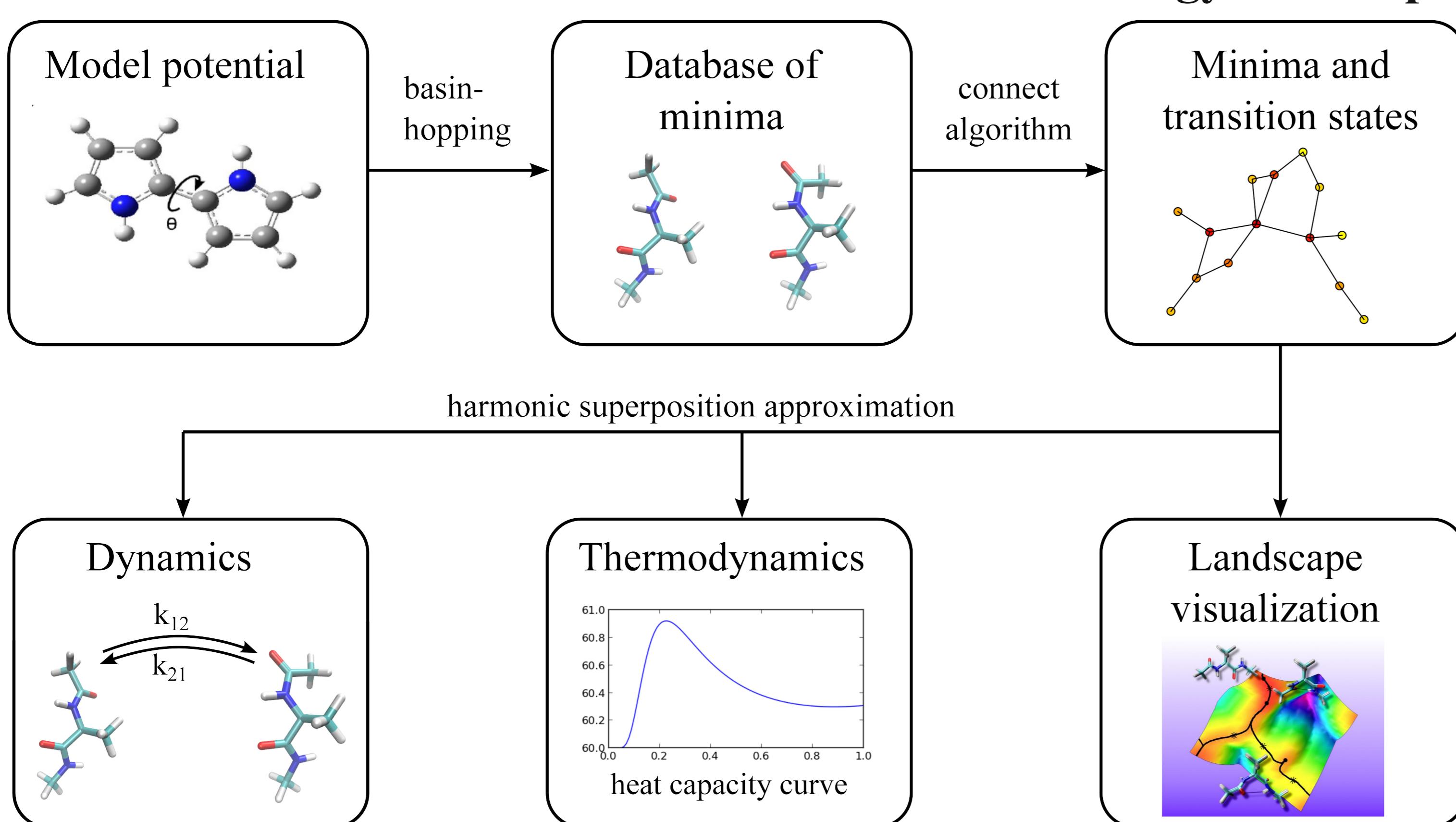
Li, Z. and Scheraga, H. A., Proc. Natl. Acad. Sci. USA, 1987, 84, 6611
 Wales, D J, and Doye J P K, Journal of Physical Chemistry A, 1997, 101, 5111.

Basin-hopping global optimization workflow



Basin-hopping corresponds to sampling on a transformed landscape

Energy landscape exploration



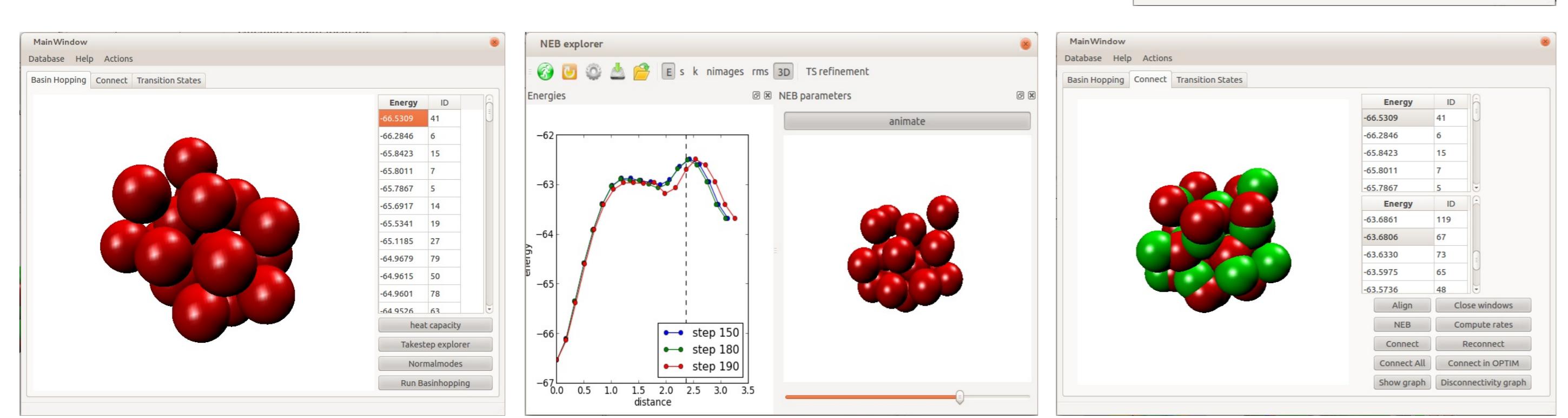
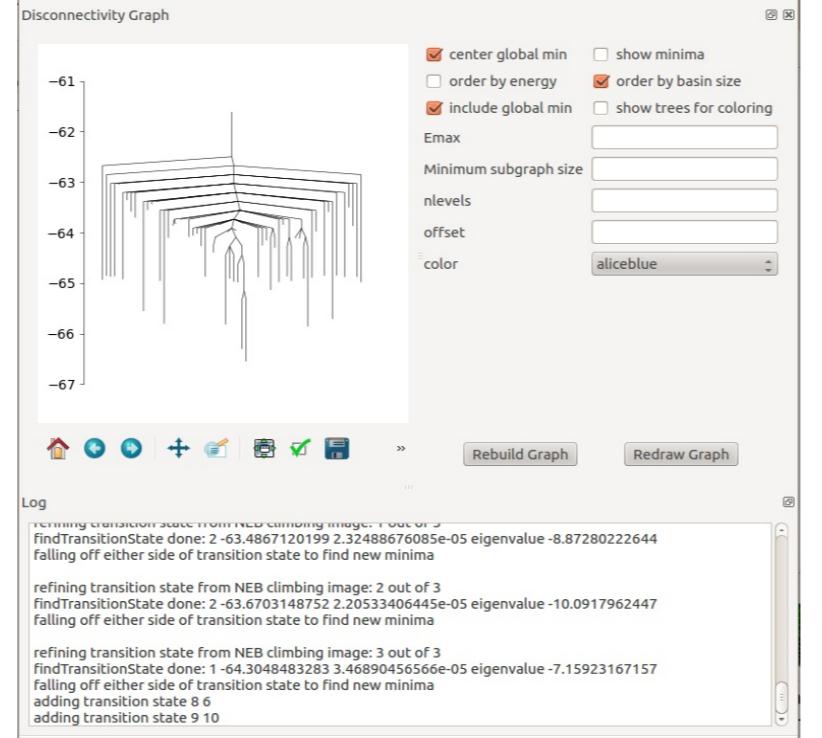
D. J. Wales, Energy Landscapes, Cambridge University Press (2004)

- The connect routine uses a modified local optimization algorithm to find transition states connecting local minima
- A disconnectivity graph visualizes local minima and the transition barriers that connect them.
- Disconnectivity graphs can be generated for high dimensional systems
- Rates for transformation between two structures can then be calculated using kinetic Monte Carlo or a graph transformation algorithm
- The framework has been used to study clusters, self assembly, proteins, glassy systems, organic crystals, and many more

Python Energy Landscape Exploration

<https://github.com/pele-python/pele>

- Modular framework for energy landscape methods
- Interface for various systems from physics and chemistry
- Python rewrite of code released by David Wales <http://www-wales.ch.cam.ac.uk/software.html>
- SQLAlchemy backend to store simulation data
- NetworkX for graph operations
- PyQt GUI to run, explore and debug simulations



Examples

