# INTERATOMIC POTENTIALS AND OPTIMISATION METHODS

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In this lecture, analytical forms of interatomic potentials (IPs) will be introduced along with the topic of energy landscapes and how to search for atomic structures corresponding to low energy local minima.Next, the following topics will be discussed: why use IPs; examples of IPs; how to obtain suitable parameters for IPs; one-dimensional optimisations; local optimisation on the potential energy landscape based on the energy and availability of its gradient and higher derivatives; example of a free energy landscape; locally ergodic regions; global optimisation methods (basin hopping, simulated annealing, evolutionary algorithms); and examples of structure prediction. Finally, a brief overview of the use of IPs in hybrid Quantum Mechanical/Molecular Mechanical (QM/MM) simulations will be given with recent applications in catalytic and optoelectronic materials.

The methods, or algorithms have been implemented with software for molecular and materials modelling. For example, GULP (http://gulp.curtin.edu.au/gulp/) has a wide range of analytical IPs, and can be used for fitting of the IP parameters, relaxing an atomic structure to the local potential energy minima and for calculating physical properties; WHAT-IP (in-house code by Scott M. Woodley) facilitates the exploration and mapping of the "fitness function" employed to refine IP parameters; KLMC (in-house code; see DOIs: 10.1021/jp406854j and 10.1039/c6nr09072a) has several global optimisation algorithms and, when used for structure prediction, automates the workflow of required structural relaxations and energy calculations performed by a third party code like GULP; HIVE (https://hive.chem.ucl.ac.uk/) is an online database of published predictions of lowest energy atomic structures of clusters; and SAINT (https://saint.chem.ucl.ac.uk/) is an online set of tools and a database to assist researchers who want to model surfaces and their reactivity to molecules. The hybrid QM/MM methods are readily available, for example, in the open-source ChemShell software (https://www.chemshell.org/). A brief overview of some of these software packages will be presented, which were also employed to generate many of the examples given in the slides.

For an introduction to this topic as applied to predicting the atomic structure of nanoclusters, see "Introduction to Modeling Nanoclusters and Nanoparticles" In: Computational Modelling of Nanoparticles, Edited by: Bromley ST, Woodley SM Source: Frontiers of Nanoscience; Series Editors: Palmer RE; Johnston, RL; Volume: 12 Pages 1-54". For reviews on structure prediction see "Crystal structure prediction from first principles" by S.M. Woodley and R Catlow in Nature Materials (Volume: 7 Issue: 12 Pages: 937-946 Year: 2008) and/or "Structure prediction of crystals, surfaces and nanoparticles" by S.M. Woodley, G.M. Day, and R. Catlow in Phil. Trans. R. Soc. A (Volume: 378 Issue: 2186 No: 20190600 Pages: 1-23 Year: 2020). For an introduction in the hybrid QM/MM methodology used see "Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches" by C.R.A. Catlow, J. Buckeridge, M.R. Farrow, A.J. Logsdail, A.A. Sokol; In: Handbook of Sold State Chemistry, edited by R. Dronskowski, S. Kikkawa, A. Stein, Wiley-VCH: Weinheim, Germany, 2017; Vol. 5, pp 647– 680 DOI: 10.1002/9783527691036.hsscvol5012. A review of the latest development in ChemShell can be found here: "Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment" by Y. Lu,M.R. Farrow, P. Fayon, A.J. Logsdail, A.A. Sokol, C.R.A. Catlow, P. Sherwood, and T.W. Keal in J. Chem. Theory Comput. (Volume: 15 Issue: 2 Pages: 1317-1328 Year: 2019).