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Is it Time to Switch to Machine Learnt Potentials?

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For over two decades I have been developing new interatomic potentials, e.g., implemented the AOM within GULP that can be employed to model non-spherical Jahn Teller Mn(III) ions, successfully refined potential parameters to model numerous systems including the Peierls' phase transition of VO₂, and I am the author of a published interatomic potential parameter database. My interest is driven by the ability to control what physics is included (or not) by the introduction of new terms to the Hamiltonian (or potential energy) and it is an approach many will follow as, compared to DFT, it allows for modelling systems of larger sizes (more atoms), greater time periods (in MD), and more sampling (global optimisation and/or calculating the partition function).

Now ML potentials, which have many more parameters to refine and a minefield of differing functional forms to choose, have become very topical as data required to fit these as well as computer resources have become more readily available. My first real experience came with one of my earlier PhD students discovering that it was not straightforward to develop a suitable model (fit parameters), for example, the GAP ML potentials we have refined suffered from the erroneous oscillations.

I lead UK's Materials Chemistry Consortium and one of our current aims is to make the use of ML potentials more accessible to our community. Simultaneously, other groups have begun refining ML-Potential models for the entire Periodic table based on reproducing DFT results. In my presentation I will present results from three of my PGT students who worked on energy materials using the JANUS-core code to calculate the energy and forces, based on pre-refined MACE ML-Potentials. Moreover, I will include recently published results on dense and microporous silica materials where these potentials performed particularly well and further results of ongoing research from the MCC.

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No. Not a student nor Postdoc.

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