Uncertainty Quantification for the Silicon GAP model



XXXXX

Complex chemistry & realistic systems...

... require large systems, long timescales and quantification of uncertainty





Challenges and Opportunities

- Propagate uncertainty on GAP atomic energies through to material properties
- UQ so far only accounts for limited training data, but there are many other sources of uncertainty – e.g. QM model error, algorithmic uncertainty, ...
- Model error: sample ensemble of "reasonable" potentials from GP without training
- Carry out active learning using predicted uncertainties to build models on-the-fly – e.g. Z. Li, J. R. Kermode and A. De Vita, *Phys. Rev. Lett.* 114 096405 (2015)
- Stochastic coarse graining to inform hierarchical multiscale models
- UQ needed for concurrent QM/MM multiscale schemes

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