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Exchange-Correlation Functional with Uncertainty Quantification Capabilities for Density Functional Theory

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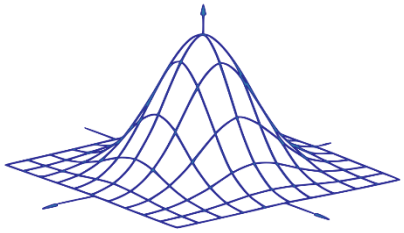
D202 Seminar room, School of Engineering, 2nd Floor

Abstract: In the last several decades, density-functional theory (DFT) has become the most widespread framework to study materials from a fully quantum-mechanical perspective due to the favourable trade-off between accuracy and computational cost it provides. Even though the theory in principle is exact, its application calls for the use of approximations, some because of computational reasons, such as the Born-Oppenheimer approximation, and some because the exact term is not known, as is the case with the exchange-correlation (XC) energy. Even though the accuracy of the different approximations has been tested in many fields, the error that they lead to when DFT is applied to new systems remains a concern, which limits the predictive power for new systems.
In this presentation, we show the development of a new meta-GGA exchange-correlation functional with uncertainty quantification capabilities from the point of view of machine learning using a Bayesian framework. The resulting functional is then used to predict quantities such as cohesive energies, lattice constants and bulk moduli including error bars stemming from our limited training data set and the inability of the model to reproduce exactly experimental results.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars



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