NANOSCIENCE COLLOQUIUM

Designing Functional Materials: Dream, Predict, Synthesise, Characterise, Repeat

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Abstract: At the Chair in Computational Materials Design, we combine computational materials design with advanced synthesis and characterisation to develop materials and interfaces, primarily for electrochemical applications. In this talk, I will present a selection of our activities in the last couple of years spanning diverse areas such as electrocatalysis, battery materials, predictive synthesis and tribology. I will also show how new theoretical developments allow us to study nano-scale systems with full atomistic detail at the Density-Functional-Theory level whilst also taking the environment into account, using the nucleation of Li clusters on graphite as example. Finally, I will provide an update on our new combinatorial physical-vapour-deposition cluster tool, which will soon allow us to tightly integrate computational materials design with combinatorial synthesis and characterisation.

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