Department of Physics
Condensed Matter Physics
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UNIVERSITY OF OXFORD

CONDENSED MATTER PHYSICS SPECIAL SEMINAR

Monday 2 March at 14:30
Simpkins Lee Seminar Room, Department of Physics
(https://maps.app.goo.gl/WjG71uLF2D48n85B6)

Hydrogen storage and production: first-principles simulations accelerated with machine learning

Professor Gabriel Antonius
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Hydrogen may serve as a carbon-free energy vector to propel electric vehicles coupled with fuel cells. The efficiency of this technology is limited by the storage and production of green hydrogen, which can be enhanced by functional materials. I will present first-principles methodologies based of density functional theory (DFT) to describe the catalytic activity of molecular complexes for the hydrogen evolution reaction, as well as the hydrogen storage properties of intermetallic compounds. In molecular complexes, the computation of Gibbs free-energy allow us to predict the most favorable catalytic pathways, the operating conditions, and the most relevant indicators for the hydrogen production rate. Then, we simulate the hydrogen storage properties of intermetallic compounds using a kinetic Monte Carlo model with DFT calculations. We show that both hybrid exchange-correlation functionals and zero-point energy corrections are necessary to obtain accurate absorption properties. Finally, I will present hybrid methods that combine DFT with molecular dynamics based on machine-learning interatomic potentials, and allow us to achieve highly efficient samplings in the canonical and grand-canonical ensembles.

Host: Professor Marina Filip