

Nicholas Hine

Nicholas Hine gained an MPhys degree from Merton College, Oxford, in 2004. His MPhys project explored computational modelling of laser-plasma interactions, and he subsequently worked briefly with the High Power Laser Group at Oxford. He started a PhD with the Condensed Matter Theory Group at Imperial College, London, in 2004 on Quantum Monte Carlo methods, where his research encompassed the application of QMC to both model systems and real materials. Since completing his thesis in 2007, he has been working as a Postdoc at the Departments of Materials and Physics at Imperial, undertaking research in Linear-Scaling Density Functional theory. He is based in the cross-disciplinary Thomas Young Centre for Theory and Simulation of Materials.

Nicholas's research focuses on the combination of thermodynamics with large-scale ab initio materials modelling. His interests lie in bridging the gap between computational theory and experiment using coherent frameworks free from empirical parameters. To this end, his recent work has involved modelling of defect formation energies in metal oxides with Density Functional Theory, and self-consistent determination of defect concentrations in real materials as a function of thermodynamic formation conditions. He also works on methodological development of Linear Scaling DFT, as one of the main contributors to the ONETEP code, and has interests in the application of many-body methods to real materials problems.

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