Daniel Mason

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Bio

After gaining a Physics degree in 1998 from St. Johns College Cambridge, Daniel Mason joined the UK national Defence Evaluation and Research Agency in Farnborough, starting his career in materials modelling with density functional theory calculations. His DPhil was awarded in 2003 by the Department of Materials Science at Oxford University for a thesis on kinetic Monte Carlo simulation of phase transformations in metals, supervised by Adrian Sutton. This then lead to post-doctoral research into using computational steering to tune Monte Carlo simulations with coarse-grained polymer models. Since October 2005, he has been researching non-adiabatic tight-binding simulations of radiation damage in metals at Imperial College London. He is also currently a member of the cross disciplinary Thomas Young Centre for Theory and Simulation of Materials.

interests

Daniel's research spans the length and time scales of materials modelling, from electronic structure calculations through molecular dynamics to kinetic Monte Carlo and coarse-grained models. He has developed accelerated computational methods for all of these, always with a clear focus on addressing real technological questions. He is currently studying irreversible energy transfer from ions to electrons in radiation damage cascades in metals. The rate at which energy can be conducted away from the damaged region is critical in determining the residual defect population, and consequently the lifetime of an irradiated structural component. This work necessitates a quantum mechanical description of the electrons beyond the Born-Oppenheimer approximation, with tens of thousands of moving atoms. He has developed a new parallel time-dependent tight-binding code, and is now using this to rigorously test the phenomenological and simplified models used in molecular dynamics simulation.