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The group is a partner, with related activities at Imperial College and University College London, in the Thomas Young Centre for Theory and Simulation of Materials. Its research is supported by a number of computer clusters housed in a dedicated server room including a 480-processor HPC cluster.

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Title:28th Workshop on Computer Simulation Studies in Condensed Matter Physics (CSP 2015) Desc:Proceedings of a meeting held 19-21 February 2015, New Orleans, Louisiana, USA. Series:Physics Procedia Volume 68 Editor:Landau, D. et al.

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The purpose of this chapter is to illustrate the basic principles underlying the current standard methods to accurately solve Eq. (1.3), which represents the main task for the ab initio calculations of the electronic structure in real poly-atomic systems. The different schemes to achieve this goal can be

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A model potential-energy function comprising both two- and three-atom contributions is proposed to describe interactions in solid and liquid forms of Si. Implications of this potential are then explored by molecular-dynamics computer simulation, using 216 atoms with periodic boundary conditions. Starting with the diamond-structure crystal at low temperature, heating causes spontaneous ...

Computer simulation of local order in condensed phases of ...

(1988). A model for the computer simulation of chemical reactions in the condensed phase. *Molecular Physics*: Vol. 65, No. 5, pp. 1153-1169.

A model for the computer simulation of chemical reactions ...

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presentations made during the 18th Annual Workshop on Computer Simulations Studies in Condensed Matter Physics at the Center for Simulational Physics at the University of Georgia in March 2005.

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