Materials structure prediction from first principles

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Abstract

The use of stochastic optimisation strategies to identify low energy configurations in the first principles energy landscape of collections of atoms is now well established. The methods used are diverse, and sometimes rather complex. Ab Initio Random Structure Searching (AIRSS), [1,2] in which initial starting structures are randomly generated (with varying degrees of preparation) and relaxed to the nearest local energy minimum repeatedly, is extremely simple and reliable. There are now many examples of these techniques making genuine computational, and scientific, discoveries, particularly in the field of high-pressure physics and increasingly in materials science. I will discuss some of these, and attempts to describe common defects, such as grain boundaries, in "realistic" materials.[3]

[1] C.J. Pickard and R.J. Needs, Phys. Rev. Lett. 2006, 97, 45504
[2] C.J. Pickard and R.J. Needs, J. Phys.: Condens. Matter Topical Review 2011, 23, 053201
[3] G. Schusteritsch, C. J. Pickard, Physical Review B, 90(3), Article No. 035424 (2014)

Biography

Chris Pickard is the inaugural Sir Alan Cottrell Professor of Materials Science in the Department of Materials Science and Metallurgy, University of Cambridge. Previously he was Professor of Physics, University College London (2009-2015), and Reader in Physics, University of St Andrews (2006-2008). He has held both EPSRC Advanced and Leadership Research Fellowships, and is currently a Royal Society Wolfson Research Merit Award holder (2015). He is a lead developer of the widely used CASTEP code, and introduced both the GIPAW approach to the prediction of magnetic resonance parameters and Ab Initio Random Structure Searching (AIRSS). In 2015 he won the Rayleigh Medal and Prize of the Institute of Physics.