凝聚态物理-北京大学论坛

Complementary approaches to the first principles calculation of phase transitions

Prof. Dario Alfe

Prof. Dario Alfe， Prof. Dario Alfe obtained his doctoral degree from SISSA, Trieste, in 1997. After that, he carried out 3 years postdoc in U.K. and became a Royal Society University Research Fellow in University College London (UCL) in 2000. In 2006, he started to work on his current position as a Professor of Physics at a very early age, in UCL. His researches mainly focus on methodology studies, ranging from electronic structures (QMC) to molecular dynamics in the computer simulation of condensed matter properties. In 2007, he was awarded the Royal Society Wolfson Research Merit Award for his contribution in these areas. Currently, he has published over 130 refereed papers, including 6 in Science or Nature, and his H-index is 37..

Abstract： Phase transitions are ubiquitous in nature, from the freezing and evaporation of water on the Earth's surface, to the solid-liquid equilibrium of iron alloys in the Earth's core, or solid-solid transitions in the Earth's mantle. For the latter, they provide a proxy to establish the pressure-temperature conditions at various depths of our planet. In the case of iron in the core, for example, we know from seismology that the solid-liquid transition is at a pressure of 329 GPa (~ 5200 km depth), and therefore knowledge of the temperature of this transition provides information on the temperature of the Earth's core, something which is otherwise impossible to measure. Phase stability is thermodynamically determined by the free energy of the system, the knowledge of which therefore provides a natural approach to the study of phase transitions. In this presentation I will discuss the method of thermodynamic integration to compute the free energies of solids and liquids. I will show how a hierarchy of methods of progressively higher accuracy can be used to obtain free energies with almost full quantum mechanical accuracy. I will show applications to several systems, including iron in the Earth's core and several other systems, which show that first principles calculations of phase transitions have now reached a degree of accuracy which competes with experiments. I will also describe other complementary approaches to the calculation of phase transitions, namely the coexistence approach and, if time permits, the recently proposed Z method. I will then conclude by discussing the main advantages and disadvantages of each of the methods.

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