凝聚态物理-北京大学论坛

2013年第12期（No.287 since 2001）

Random search-a tool for physics discovery

Prof.Chris J.Pickard

时间：5月30日（星期四）15:00—16:40

地点：北京大学物理大楼中212教室

About speaker The research interests of Prof. Chris J. Pickard range from theoretical high pressure physics to the study of pharmaceutical compounds using combined theoretical and experimental solid state NMR. His approach is atomistic, using so-called first principles techniques to quantum mechanically describe the interaction between the electrons and nuclei which make up minerals or drug molecules. He is an electronic structure theorist and a lead developer (responsible for the underlying pseudopotential technology) of the widely used CASTEP code. Recently he has introduced the strikingly simple, and effective, Ab Initio Random Structure Searching (AIRSS) approach to materials structure prediction.

Abstract: Much progress has been made in the prediction of structure from first principles. Professor Chris J. Pickard uses the method- Ab Initio Random Structure Searching (AIRSS)[1,2], which is simple and powerful. Its lack of bias makes it particularly suitable for theoretical explorations leading to new and unexpected phenomena. He has uncovered ionic phases of ammonia[3], and structural richness at terapascal pressures in Aluminium[4] and Iron[5].This presentation focuses on the hunt for novel physics, illustrated by the discovery of a new route to bulk magnetism in the elements[6] and the decomposition of water under terapascal conditions.[7]

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[2] C.J. Pickard and R.J. Needs, J. Phys.: Condens. Matter Topical Review 2011, 23, 053201
[3] C.J. Pickard and R.J. Needs, Nature Materials 2008, 7, 775-779
[4] C.J. Pickard and R.J. Needs, Nature Materials 2010, 9, 624-627
[5] C.J. Pickard and R.J. Needs, J. Phys.: Condens. Matter 2009, 21, 452205
[6] C.J. Pickard and R.J. Needs, Phys. Rev. Lett. 2011, 107, 087201
[7] C.J. Pickard, Miguel Martinez-Canales, and R.J. Needs, Phys. Rev. Lett. 2013 (accepted)