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Random search - a tool for exploring dense matter¹

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There has been great progress in the prediction of structure from first principles - thanks to the combination of stochastic search algorithms with reliable density functional based evaluations of the energy landscape. My approach - Ab Initio Random Structure Searching (AIRSS) [1,2] is particularly simple and powerful. In its most straightforward implementation, a lack of bias makes it suitable for theoretical explorations which can lead to new and unexpected phenomena. I have uncovered ionic phases of ammonia [3], and structural richness at terapascal pressures in aluminium [4]. An emphasis has been placed on the hunt for novel physics, illustrated by the discovery of a new route to bulk magnetism in the elements [5] and the decomposition of water under terapascal conditions [6]. The imposition of geometrical constraints permits the directed search for the ground state structure of complex compounds - I will discuss the application of AIRSS to the computational discovery of new materials.

[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] 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, Phys. Rev. Lett. 2011, 107, 087201.

[6] C.J. Pickard, Miguel Martinez-Canales, and R.J. Needs, Phys. Rev. Lett. 110, 245701 (2013)

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