Random search - a tool for exploring dense matter

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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) \cite{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 \cite{3}, and structural richness at terapascal pressures in aluminium \cite{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 \cite{5} and the decomposition of water under terapascal conditions \cite{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.


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