MAR16-2015-020246 C

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Discovering new materials and new phenomena with evolutionary algorithms

ARTEM OGANOV, Skolkovo Institute of Science and Technology

Thanks to powerful evolutionary algorithms, in particular the USPEX method, it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increases of efficiency and extensions to low-dimensional systems and molecular crystals (which allowed large structures to be handled easily, e.g. $Mg(BH_4)_2$ and H_2O-H_2) and new techniques called evolutionary metadynamics and Mendelevian search. Some of the results that I will discuss include: 1. Theoretical and experimental evidence for a new partially ionic phase of boron, γ-B and an insulating and optically transparent form of sodium. 2. Predicted stability of "impossible" chemical compounds that become stable under pressure – e.g. Na_3Cl, Na_2Cl, Na_3Cl_2, $NaCl_3$, $NaCl_7$, Mg_3O_2 and MgO_2. 3. Novel surface phases (e.g. boron surface reconstructions). 4. Novel dielectric polymers, and novel permanent magnets confirmed by experiment and ready for applications. 5. Prediction of new ultrahard materials and computational proof that diamond is the hardest possible material.