Prediction of complex high-pressure M-B crystal structures with an evolutionary algorithm

ALEKSEY KOLMOGOROV, SHEENA SHAH, ROXANA MARGINE, University of Oxford — We have carried out an ab initio ground state search in two binary metal-boron systems using an evolutionary algorithm [1] and identified remarkably complex configurations stabilized at high pressures [2,3]. An alkali-earth metal boride is shown to undergo a structural transformation from a semiconducting to a metallic state while a new semiconducting transition metal boride is stabilized at a composition known to have only metallic ground states. For the proposed candidate materials we calculate the electron-phonon coupling and demonstrate their potential to be phonon-mediated superconductors.