

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

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.

[1] A.N. Kolmogorov, <http://maise-guide.org> (MAISE)

[2] A. N. Kolmogorov, S. Shah, E. R. Margine, A. F. Bialon, T. Hammerschmidt, R. Drautz, Phys. Rev. Lett. 105, 217003 (2010).

[3] A. F. Bialon, T. Hammerschmidt, R. Drautz, S. Shah, E. R. Margine, A. N. Kolmogorov (submitted)

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Date submitted: 27 Dec 2010

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