Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Generation and analysis of the largest ab initio database for metal borides ABRAM VAN DER GEEST, ALEKSEY KOLMOGOROV, Binghamton University - SUNY — Boron-based materials have been observed in a remarkable variety of crystal structures with outstanding superconducting, mechanical, and refractory properties. Aiming to provide a systematic description of known compounds and to identify new synthesizable candidate materials, we have generated an extensive ab initio database spanning over 40 binary and ternary metal boride systems at ambient and gigapascal pressures. The considered crystal structures include known prototypes listed in the ICSD as well as brand-new prototypes found with an evolutionary search implemented in MAISE [1]. Having examined over 15,000 entries of calculated formation enthalpies, we find a number of surprising disagreements between theory and experiment regarding the ground state crystal structures and identify over a dozen systems in which novel compounds are expected to form under high pressures. Data mining of the ab initio information has revealed trends in the electronic, magnetic, vibrational, and elastic properties which can help fine-tune the metal boride materials for specific applications. [1] Module for Ab Initio Structure Evolution, http://maise-guide.org

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Date submitted: 09 Nov 2012 Electronic form version 1.4