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Prediction and confirmation of new MB4 crystal structures (M=Cr,Fe,Mn) ABRAM VAN DER GEEST, ALEKSEY KOLMOGOROV, State University of New York - Binghamton University, KOLMOGOROV GROUP TEAM — The family of $3d$ transition metals tetraborides has recently attracted a lot of interest due to the materials' unusual structural, mechanical, and superconducting properties [1-6]. We overview our computational work on the determination of their ground state structures and show that all the predictions have been confirmed by experimental groups. Namely, the true ground state of the known CrB_4 and MnB_4 compounds have been determined to be new orthorhombic and monoclinic structures, as predicted by a combination of high-throughput and evolutionary searches [3,6,7]. The proposed brand-new FeB_4 superconducting compound [3] has been synthesized by our colleagues and shown to be a superhard superconductor [4,5]. We discuss the possibility of raising the material's superconducting critical temperature by doping. [1] A. N. Kolmogorov, S. Shah, et al., Phys. Rev. Lett., 105, 217003. [2] A. F. Bialon, T. Hammerschmidt, et al., Appl. Phys. Lett., 98 081901. [3] H. Niu, J. Wang, et al., Phys. Rev. B, 85, 144116. [4] H. Gou, N. Dubrovinskaia, et al. Phys. Rev. Lett., 111, 157002. [5] Filip Ronnig and John L. Sarrao, Physics 6, 109 (2013). [6] A.G. Van Der Geest and A. N. Kolmogorov, ArXiv: http://xxx.lanl.gov/abs/1310.4157 . [7] MAISE http://maise-guide.org .

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