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Theory-guided discovery of new superconducting materials[1]

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Extensive theoretical effort to predict new superconductors has resulted in remarkably few discoveries. Successful examples so far have been restricted primarily to pressure- or doping-driven superconducting transformations in existing materials. In this talk I will describe our work that has led to the prediction [1] and discovery [2] of a brand-new superconducting FeB4 compound with a previously unknown crystal structure. First measurements supported the predicted phonon-mediated pairing mechanism, rare for an iron-based superconductor. The identification of FeB4 candidate material was a result of combined high-throughput screening, targeted evolutionary search [3], and rational design. The systematic study of more than 12,000 metal boride phases has identified dozens of synthesizable materials with unusual structural motifs, some of which have been confirmed experimentally [4]. I will overview employed strategies for selecting promising superconducting compounds and describe our on-going work on accelerating the search for stable materials. [1] A.N. Kolmogorov *et al.*, Phys. Rev. Lett. 105, 217003 (2010) [2] H. Gou *et al.*, Phys. Rev. Lett., 111, 157002 (2013) [3] Module for Ab Initio Structure Evolution (2009-), http://maise-guide.org [4] A.G. Van Der Geest and A. N. Kolmogorov, CALPHAD 46, 184 (2014)

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