Theory-guided discovery of new superconducting materials

ALEKSEY KOLMOGOROV, Binghamton University, SUNY

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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