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Materials design with high-throughput computing: metal borides.

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The search for stable candidate materials with new properties poses a number of challenges, from sampling large configuration spaces of structures and compositions to demonstrating the validity of the chosen simulation method. I will present the results of two extensive computational studies that highlight the necessity (i) to go beyond standard structure types even for binary systems under normal conditions and (ii) to go beyond the standard density functional theory (DFT) approximations to describe a seemingly ordinary class of metal borohydrides. In the first case, application of an ab initio evolutionary search has uncovered unusual TM-B candidate materials stable under ambient pressure with potential for superconductivity and hard coating applications [1]. In the second case, inclusion of nonlocal correlation effects within van der Waals DFT has resolved an outstanding discrepancy between theory and experiment regarding the low-temperature ground state of Mg(BH4)2 [2].

[1] A.N. Kolmogorov, S.Shah, E.R. Margine, A. Bialon, T. Hammerschmidt, and R. Drautz, submitted (2010).
[2] A. Bil, B. Kolb, R. Atkinson, D.G. Pettifor, T. Thonhauser, and A.N. Kolmogorov, submitted (2010).