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First Principles Search for New Superconducting Layered Borides

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The identification of novel crystal structures is a fundamental step for predicting new stable compounds in alloys. While performing ab initio data mining of intermetallic compounds [1], we discover a new family of layered metal borides [2], of which MgB_2 is one particular element (the new phases are called Metal Sandwich (MS)). Thermodynamic stability and electronic properties of these MS phases are investigated in details, leading to the prediction of a hypothetical novel superconductor MS-LiB [2,3]. Calculations show that the MS phases in the Li-B system exhibit electronic features similar to those of MgB_2 [2,3] and CaC_6 [4]. Although the predicted critical temperature of LiB is lower than that of MgB_2 (references [4] and [5] for MS2-LiB and MS1-LiB, respectively), the peculiarities of MS-LiB in terms of electronic structure, layer arrangements and doping capabilities allow a lot of freedom in the search for higher T_c systems [5,6]. We acknowledge the Teragrid-Partnership for computational resources. Research supported by ONR and NSF. [1] Phys. Rev. Lett. **9**1, 135503 (2003). [2] Phys. Rev. B **73**, 180501(R) (2006). [3] Phys. Rev. B **74**, 224507 (2006). [4] Phys. Rev. B **75**, 064510 (2007). [5] Phys. Rev. B **75**, 144506 (2007). [6] A. N. Kolmogorov, M. Calandra, and S. Curtarolo, *Engineering superconductors with ab initio methods: ternary metal borides*, (2007).