Engineering superconductors with ab initio methods: the example of LiB
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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]. We acknowledge the San Diego Supercomputer Center for computational resources.