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Combining the advantages of superconducting MgB2 and CaC6 in one material: suggestions from first-principles calculations AMY LIU, Georgetown University, IGOR MAZIN, Naval Research Laboratory — We show that a recently predicted layered phase of lithium monoboride, Li_2B_2, combines the key mechanism for strong electron-phonon coupling in MgB_2 (i.e., interaction of covalent B σ bands with B bond-stretching modes) with the dominant coupling mechanism in CaC_6 (i.e., interaction of free-electron-like interlayer states with soft intercalant modes). Yet, surprisingly, the electron-phonon coupling in Li_2B_2 is calculated to be weaker than in either MgB_2 or CaC_6. This is due to the accidental absence of B π states at the Fermi level in Li_2B_2. In MgB_2, the π electrons play an indirect but important role in strengthening the coupling of σ electrons. We discuss the use of doping to restore π electrons at the Fermi level, which would enhance the coupling and the superconducting T_c.

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