

Abstract Submitted
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Light element ternary compounds – searching for new superconductors in the “upper left corner”¹ ANDREAS HERMANN, NEIL W. ASHCROFT, ROALD HOFFMANN, Cornell University — We propose here a new class of ternary compounds, composed entirely of light elements drawn from the upper left corner of the Periodic Table, as a new family of superconductors with the promise of high transition temperatures (T_c). In this explorative computational study, we have investigated stoichiometric 1:1:1 compounds of lithium, beryllium, and boron. We find layered metallic phases that are thermodynamically stable at $P=1$ atm, with still others stabilized at relatively low pressures and hence in principle accessible to synthesis and experimental characterization. At high pressures, close packed structures are again stabilized and a metal-to-insulator transition is predicted. Superconducting transition temperatures for the most structurally attractive metallic phases are estimated using BCS theory. An outlook on other stoichiometries, as well as the incorporation of different constituents, Mg instead of Be in particular, is given.

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