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Tuning dimensionality in binary Li-B compounds and evaluating thermodynamic vs kinetic stability under pressure[1] ANDREAS HERMANN, Cornell University — The binary phase diagram of the light elements lithium and boron features an intriguing phase with a finite range of stability, LiB_x with $0.8 \leq x \leq 1.0$. The experimental hexagonal structure contains two incommensurate sub-lattices, a hexagonal lithium network, and an array of linear boron chains. An alternative structure of almost equal energy is inspired by the AlB_2 structure type, and contains graphitic boron sheets interspersed by trigonal lithium layers. We present results from a computational study on this system, at atmospheric and elevated pressures. We model the tunable atomic composition and predict the disappearance of the finite stability range of LiB_x at P=40GPa, where layered structures become more stable than chain-like structures across the entire composition range. Kinetic barriers are estimated and are predicted to facilitate the recovery of phases synthesized at high pressure. Up to P=70GPa, all stable structures are metallic, and trends of their electronic and dynamic properties will be discussed. At P>70GPa, structure searches reveal that stoichiometric 1:1-LiB is most stable in the NaTl structure, with a diamondoid boron network, and becomes an insulator. The Zintl-Klemm concept helps understand the different structural choices under pressure.

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