Quasi-two-dimensional electronic states in a dense three-dimensional Li-Be alloy

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High pressure can affect electronic structure and crystal packing, and in some cases even induce compound formation between elements that do not bond under ambient conditions. Our computational study for the Li-Be system shows that the reactivity of Li and Be is fundamentally altered by pressure. These two lightest of all metallic elements are immiscible at ambient conditions. Using structure search methods[1,2] we discover four stoichiometric $Li_x\ Be_{1-x}$ compounds that are stable over a range of pressures.[3] The electronic density of states of one of them displays a remarkable step-like feature and plateau at the bottom of the valence band, which is typical of a quasi-2D electronic structure and rather unexpected in a 3D crystal environment. We attribute this feature to large size differences between the ionic cores of Li and Be. Under increased pressure, the Li cores start to overlap and thereby expel valence electrons into quasi-two-dimensional layers characterized by delocalized free-particle-like states in the vicinity of Be ions. These alloys are also interesting from the perspective of superconductivity. The T_c in the LiBe alloy is expected to be substantially higher than that of the component elements due to the increased density of states at the Fermi energy compared particularly to elemental Be.

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[2] D. G. Pettifor. *A Chemical Scale for Crystal-Structure Maps* . Solid State Commun. **51**, 31 (1984).

[3] J. Feng, R. G. Hennig, N. W. Ashcroft and Roald Hoffmann. *Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys.* Nature **451**, 445 (2008).