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Exploring superconductivity of the $(Hf_{0.2}Mo_{0.2}, Ta_{0.2}, Nb_{0.2}, Ti_{0.2})B_2$ high entropy alloy and its metal diborides: The effect of adsorbed hydrogen

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Interest in 2D superconducting materials has been gaining momentum in recent years due to its potential applications for nanoscale devices such as superconducting transistors, quantum interferometers, and superconducting qubits. In particular, a family of materials known as layered hexagonal metal borides (MB_2) has garnered intrigue as a probe for investigating the behaviour of superconductivity at the 3D to 2D transition. This is due to the fact that many of these MB_2 compounds are chemically exfoliable from single-crystalline layered ternary borides. Numerous MB_2 compounds have been shown experimentally to be superconducting in bulk form. Among them MgB_2 has demonstrated the highest electron-phonon mediated superconducting transition temperature ($T_c = 39$ K) at ambient pressure to date. Furthermore, MgB_2 is shown to be strongly influenced by surface states, as demonstrated by significant changes in its T_c when thinned down to monolayer thickness, as well as to surface hydrogenation of the 2D structure. Interestingly, the formation of high-entropy metal diborides have been reported. These structures are composed of 2D high-entropy metal layers, separated by 2D boron nets. They represent a new class of high-entropy materials, which are not only among the first high-entropy non-oxide ceramics fabricated, but also possess a unique non-cubic (hexagonal) and layered (quasi-2D) crystal structure.

Using density functional theory with the Eliashberg formalism we investigate phonon-mediated superconductivity in the 2D $(Hf_{0.2}Mo_{0.2}, Ta_{0.2}, Nb_{0.2}, Ti_{0.2})B_2$ high entropy alloy and its metal diborides with varying surface hydrogenation to provide insight into how different metal dopants and surface hydrogenation impact the transition temperature of these materials.

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