Hydrogen-induced high-temperature superconductivity in two-dimensional materials: The case of hydrogenated monolayer MgB_2

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In seminal work of 1968 Ashcroft showed that dense metallic hydrogen, if ever produced, could be a high-temperature superconductor, owing to its very high Debye temperature, as a result of its minimal mass, enabling very strong phonon-mediated superconducting pairing according to the Bardeen-Cooper-Schrieffer (BCS) theory [1]. Currently, it has been well established that hydrogen-based compounds under ultra-high pressure, such as the polyhydrides H_3S [2] and LaH_{10} [3,4], superconduct through the conventional electron-phonon coupling mechanism to attain the record critical temperatures (T_c) known to date.

We will demonstrate that the intrinsic advantages of hydrogen for phonon-mediated superconductivity can be exploited in a completely different system, namely two-dimensional (2D) materials [5]. Namely, we found that hydrogen adatoms can strongly enhance superconductivity in 2D materials. Firstly, Van Hove singularities in the electronic structure, originating from atomic-like hydrogen orbitals, lead to a strong increase of the electronic density of states, thus enhancing the electron-phonon coupling. Furthermore, the emergence of high-frequency hydrogen-related phonon modes in this system boosts the electron-phonon coupling further.

As a concrete example, we will focus on the effect of hydrogen adatoms on the superconducting properties of monolayer MgB_2 [6,7], which we investigated by solving the fully anisotropic Eliashberg equations, in conjunction with a first-principles description of the electronic and vibrational states, and the coupling between them. We will show that hydrogenation leads to a high T_c of 67 K, which can be boosted to over 100 K by biaxial tensile strain. This proves that hydrogenation of a 2D material can indeed induce strong electron-phonon coupling and high-T_c superconductivity, as exploited in the bulk hydride compounds with record T_c's to date [3,4], yet without the need to apply excessively high pressures that hamper practical applications.

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