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Searching for higher superconducting transition temperature in strained MgB2 using first principles calculations JIN-CHENG ZHENG, Brookhaven National Laboratory, YIMEI ZHU, Brookhaven National Laboratory
— Since the discovery of the amazing high superconducting transition temperature (T_c) in non-oxide MgB_2, great efforts have been made on the search for higher T_c in MgB_2 and related materials by either chemical substitutions or by applying pressures to modify the lattice of MgB_2. Little success has been achieved so far due to the fact that the T_c is always suppressed using either method. To tailor the T_c in MgB_2, the full atomic-level understanding of underlying mechanism of chemical and lattice effects is required. According to the McMillan-Allen-Dynes analysis, T_c in MgB_2 is controlled by the collective contributions from phonon frequency, electron-phonon coupling and Coulomb repulsion. Consideration of one single parameter alone cannot guarantee the improvement of T_c because of the strong coupling and competing of other parameters. Here we present a detailed first-principles density functional analysis of the effects of lattice strains to superconducting properties of MgB_2. On the basis of our results for structural, electronic, vibrational and superconducting properties of strained MgB_2, we show how higher superconducting transition temperature might be achieved in strained MgB_2 superconductor.

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