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Superconductivity of 2D materials with metal intercalation[1] JUN-JIE ZHANG, SHUAI DONG, Southeast University — In this report, the electronic structure and lattice dynamics of 2D materials with monolayer metal intercalated have been calculated via first-principles density functional theory and density functional perturbation theory. According to the electron-phonon interaction, it is predicted that these 2D materials can be transformed from semiconductors to superconductors by metal intercalation. More interestingly, the biaxial tensile strain can significantly enhance the superconducting temperature up to about 10 K in Na-intercalated MoS_2, and we also predicted above 20 K superconductivity in blue phosphorus bilayer. In addition, the phonon mean free path at room temperature is also greatly improved in Na-intercalated $MoSe_2$, which is advantageous for related applications.

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