Phonon-mediated superconductivity in Janus MoWX (X = C, N) MXenes

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Janus MXenes have emerged as a promising class of 2D materials with tunable structural, electronic, and superconducting properties. In this presentation, we employ first-principles calculations to investigate the structural, mechanical, and electronic properties of Janus MoWX (X = C or N) MXenes, with a particular focus on their superconducting behavior and response to biaxial strain and surface functionalization. Our findings indicate that the hexagonal (2H) phase is energetically more favorable than the tetragonal (1T) phase for both MoWC and MoWN MXenes. For Janus MoWC, the 2H phase exhibits superior mechanical strength compared to the 1T phase, withstanding up to 9% tensile strain due to the robust C–C bonding network. Notably, we identify phonon-mediated superconductivity in 2H-MoWC, with an intrinsic superconducting transition temperature (T_c) of 1.6 K, which can be significantly enhanced to 7 K under biaxial strain. In the case of Janus MoWN, oxygen functionalization plays a crucial role in stabilizing the 2H phase and enhancing its elastic properties. Both 2H and 1T-MoWNO2 exhibit metallic behavior, prompting an exploration of their electron-phonon coupling effects. Our analysis reveals a T_c of 12.0 K for 1T-$MoWNO_2$ and 2.7 K for 2H-$MoWNO_2$, demonstrating the influence of structural phase and surface termination on superconductivity. Overall, our study provides comprehensive insights into the phonon-mediated superconductivity of Janus MoWX MXenes, highlighting their tunable electronic and mechanical properties. The strain-dependent superconducting enhancement in MoWC and the functionalization-driven superconducting behavior in MoWN establish these materials as potential candidates for next-generation electronic and superconducting applications.

References

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