Engineering the Properties of 2D Carbide Structures

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As two-dimensional material become more prolific it is increasingly clear the way in which their properties strongly depend on composition, defects, and surface structure. Computational methods at the level of first-principles density functional theory calculations and atomic-scale simulations can quantify these dependencies in a way that is highly complementary to experimental data. Here, computational methods are used to investigate the structure-property dependence of two-dimensional metal carbides, carbon-doped metal dichalcogenides, and MXenes. The computational predictions are compared to experimental data to advance design of two-dimensional materials.