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Crystal Structures, Phase Stability, and Electronic Properties of Two Dimensional Ferroelectric MXenes. MO LI, JOSHUA YOUNG, New Jersey Inst of Tech — Two-dimensional ferroelectrics, or monolayer materials that display a switchable electric polarization, have attracted attention during recent years due to their advanced electronic properties that can be used in various practical applications. In addition to the widely studied 2D materials like In2Se3 or MoTe2, the MXene Sc2CO2 was also recently predicted to possess ferroelectric properties in a metastable phase. In this work, Density Functional Theory (DFT) and the Berry Phase approach were used to study both the structures and the ferroelectric properties of additional MXene materials. Eight MXenes with chemical formula M2CT2 were carefully studied, where M represents a transition metal (M = Sc, Y), Cis carbon, and T represents the surface termination group (T = O, F). We computed the phonon bandstructures and determined the monolayers are dynamically stable. The polarization and the piezoelectric tensors were calculated, and we found that Y2CO2 has a stable ferroelectric ground state and an out-of-plane polarization larger than other materials. Finally, we computed the band gap of each material and found Y2CO2 exhibits a bandgap of 2.07 eV, which gives it potential as an photocatalytic material.

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