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Computational screening of MXene-based catalysts for chlorinated hydrocarbons removal

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Chlorinated hydrocarbons such as trichloroethylene (TCE) persist in the environment and pose significant risks to human health and ecosystems. Conventional remediation techniques are often energy-intensive and inefficient, underscoring the need for innovative solutions. In this work, we employ density functional theory (DFT) to systematically investigate the catalytic potential of MXene-based materials for the dechlorination of TCE and related pollutants. Focusing on MXenes such as Sc_2C, Ti_2C, and V_2C, we explore the impact of various surface terminations (i.e., -F, -O, and -OH) as well as the role of surface defects on adsorption and catalytic activity.

Our simulations reveal that TCE adsorbs favorably on fully -O and -F terminated MXene surfaces, with adsorption energies ranging from -0.63 eV to -0.80 eV. Importantly, -OH terminated MXenes exhibit spontaneous dechlorination with zero energy barriers, while defect-induced exposed metal sites for -O and -F terminations enhance reactivity by lowering the activation barriers, as evidenced by Nudged Elastic Band (NEB) calculations (e.g., 0.07 eV on Sc2 CF2). As a realistic scenario, studies on mixed terminations demonstrate that even modest -OH coverage sustains efficient dechlorination. Other chlorinated hydrocarbons DDT and lindane show similar behavior as spontaneous dechlorination on $Ti2C(OH)_2$ extending the MXenes catalytic applicability.