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Dimensional Reduction Activates $Ti_{n+1}C_nO_2$ MXenes: Edge-Controlled Quantum Dots Enable Ultralow-Barrier Dechlorination of Trichloroethylene

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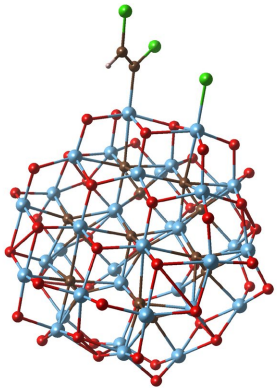

Trichloroethylene (TCE) remains one of the most persistent and mobile groundwater contaminants, demanding efficient catalytic solutions beyond conventional remediation technologies. In our previous DFT screening of MXene-based materials, we showed that extended Ti_2CO_2 surfaces interact with TCE predominantly via dispersion forces and that C–Cl bond cleavage on pristine 2D MXenes is strongly endothermic, unless defects or hydroxyl groups are introduced [1].

Here, we demonstrate that dimensional reduction fundamentally transforms the catalytic behavior of Ti-based MXenes. Using dispersion-corrected density functional theory and climbing-image NEB calculations, we investigate **$Ti_{n+1}C_nO_2$ quantum dots (QDs)** as intrinsically edge-engineered catalytic motifs. We systematically resolve the role of edge coordination, oxygen coverage, curvature, and the nanoribbon limit connecting 0D and 2D systems.

We uncover a reactivity switch upon reduction from 2D sheets to finite quantum dots. Bare-edge QDs promote spontaneous TCE dissociation without an activation barrier. Even partially oxygen-saturated edges retain ultralow activation energies, while fully saturated edges remain catalytically active with sub-eV barriers. In sharp contrast, the corresponding extended Ti_2CO_2 monolayer is catalytically inert toward TCE dechlorination.

The enhanced activity can be attributed to the presence of low-coordinated edge Ti sites that emerge upon dimensional reduction from extended sheets to finite quantum dots. These sites provide favorable geometrical environments for TCE adsorption and C–Cl bond activation, stabilizing dissociated configurations relative to the 2D limit. Comparison across small and large QDs and the nanoribbon model indicates that catalytic activity is governed primarily by edge chemistry and local coordination, rather than quantum confinement effects alone.

These results identify Ti based MXene quantum dots as intrinsically activated MXene derivatives and establish edge engineering as a powerful design principle for nanomaterials targeting chlorinated groundwater contaminants.

[1] Kolos M., Karlický F.: Computational screening of MXene-based catalysts for chlorinated hydrocarbons removal. *J. Phys-Mater. 8(3), 035001,* ***2025***

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