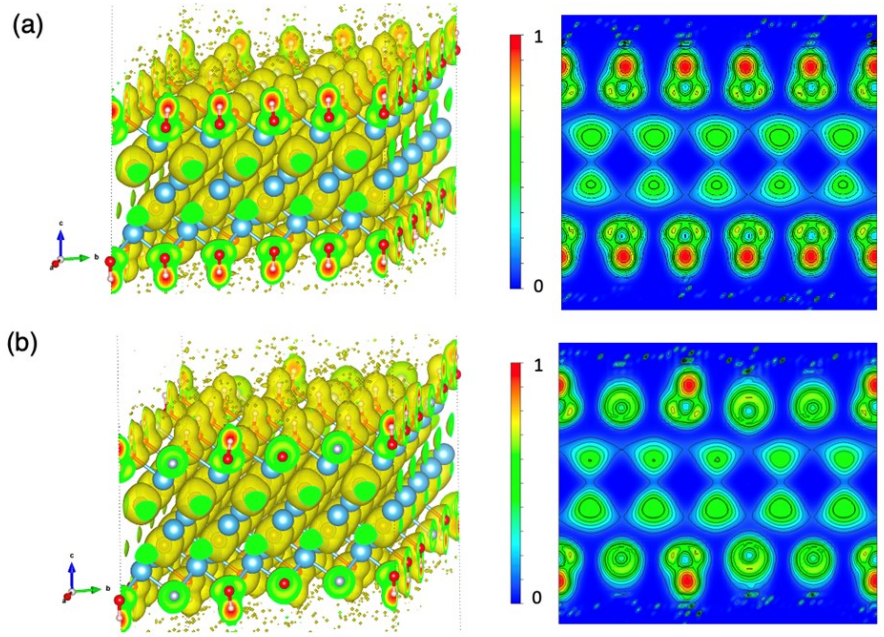
Tuning MXene Surface Terminations for Strategic Control of Physical Properties



(a) Ordered termination surface of $Ti_3C_2O_{0.24}(OH)_{1.28}F_{0.48}$.
(b) Random termination surfaces of $Ti_3C_2O_{0.24}(OH)_{1.28}F_{0.48}$.
The right panel shows a 2D slice of the electron localization function viewed from the (100) plane. Red and blue regions in the right panel represent localized and delocalized charge with an isovalue of 1 and 0 respectively.

Chu, Y. Z.; Hoover, M.; Ward, P. A.; Lau, K. C. Tuning MXene surface terminations with varying HF-concentration: A first-principles study of $Ti_3C_2T_x$. *iScience*, **2023**, accepted.

Scientific Achievement

- $Ti_3C_2T_x$ surfaces with a higher hydroxyl group concentration play a pivotal role in surface properties and were found to be thermodynamically stable.
- From the electronic bonding analysis, the charge density difference and electron localization function demonstrated a significant electron localization at the hydroxyl group, which results in a locally induced dipole on the surface.
- A large tunability in the work function is found from different concentrations of functional groups on the surface which can be controlled by the concentration of HF used for etching of the MAX phase to produce the resulting MXene.

Significance and Impact

- These results provide valuable insight into the fundamental surface characteristics of $Ti_3C_2T_x$ MXenes and a design pathway for strategically tuning the material properties through control of the HF concentration during material synthesis

Research Details

- The influence of termination group distribution on the surface of $Ti_3C_2T_x$ MXenes from various etching concentrations of HF was evaluated
- The work functions of $Ti_3C_2T_x$ MXenes with differing concentrations of functional groups were determined
- The influence of termination group clustering on the surface of $Ti_3C_2T_x$ MXenes was investigated by visualization of the electron localization function and charge density difference

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