2D MXENES AS CHEMICAL SENSORS IN THE ART MUSEUM ENVIRONMENT

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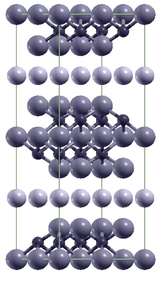
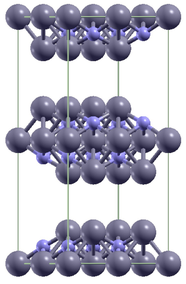
Introduction

- In 2011, a new class of materials called MXenes was discovered via HF acid etching of Al[1]
- These materials have found applications as thin films, sensors, and as biological delivery systems
- Here we investigate if they could act as sensors in the museum environment for a variety of common small molecules
- Harmful adsorptions of small molecules are a common method of degradation for works of art

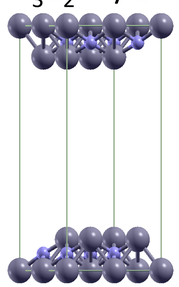
Ti_3AlC_2 MAXene



Ti_3C_2 MXene



Ti_3C_2 W/O Middle



Methods

- We use first principles atomistic Density Functional Theory (DFT), to simulate surface adsorption reactivity on MXenes
- DFT is a noninvasive probe to understand degradation mechanisms in conservation science and to design new functional materials
- To run these calculations, we use the open source planewave package Quantum Espresso and the GBRV pseudopotential set
- By choosing to either keep or remove the middle layer of our system, we can simulate either confined nanoscale (3.69 Å) or surface interaction (11.28 Å) environments, effectively probing multiple chemical environments
- A representative sample of small molecules was chosen

Goals for DFT Calculations

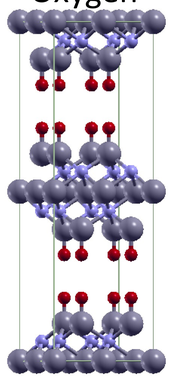
- Simulate interactions between common adsorbates in the museum environment and a Ti_3C_2 MXene layer
- Observe differences in possible terminations of Ti_3C_2 MXenes
- Calculate bond length and adsorption energies using DFT
- Consider usage of Ti_3C_2 MXenes as protective films
- Evaluate MXene sensor applications for small molecules

Results

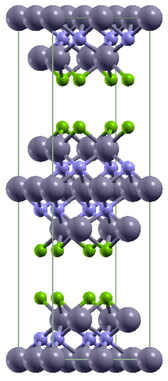
- Deprotonation occurred with ammonia and water
- Oxygen taken from SO3
- Accurate reproduction of Ti-N, Ti-F, and Ti-O bonds
- Differentiation of behavior between tetrahedral and octahedral terminations

Homogenous Ti_3C_2 Surface Terminations

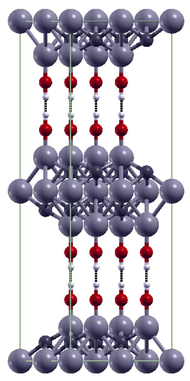
Oxygen



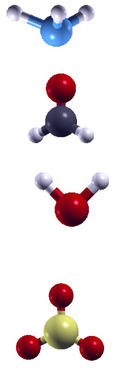
Florine



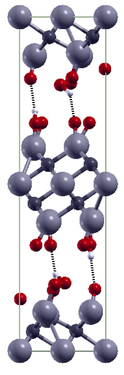
Hydroxide



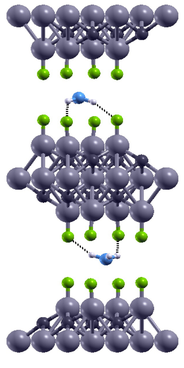
Small Molecule Adsorbates



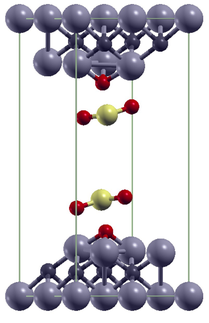
Oxygen-H_2O



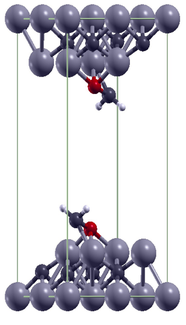
Florine-NH_3



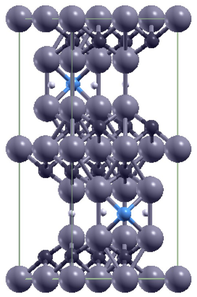
Bare-SO_3



Bare-CH_2O



Ti_3C_2 With NH_3 (deprotonated)



Adsorbate on Ti_3C_2	E_{ads}(eV)
H_2O	-10.41
NH_3	-8.87
CH_2O	-8.74
SO_3	-23.95

Bond	Bond Length (Å)	Accepted Value (Å)
Ti-F Tetrahedral	1.761	1.763[2]
Ti-F Octahedral	2.166	2.180[2]
Ti-O	1.621	1.627[3]
Ti-N	2.226	2.192[4]

Conclusions

- We were able to differentiate between octahedral and tetrahedral configurations of Florine terminations on Ti_3C_2
- Observed differences between possible terminations on Ti_3C_2, which can be probed for further analysis

References

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Acknowledgments

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