Adsorption of Selenium Oxo-anions on [012] Alumina Surface and Its Dependence on Configuration and Protonation

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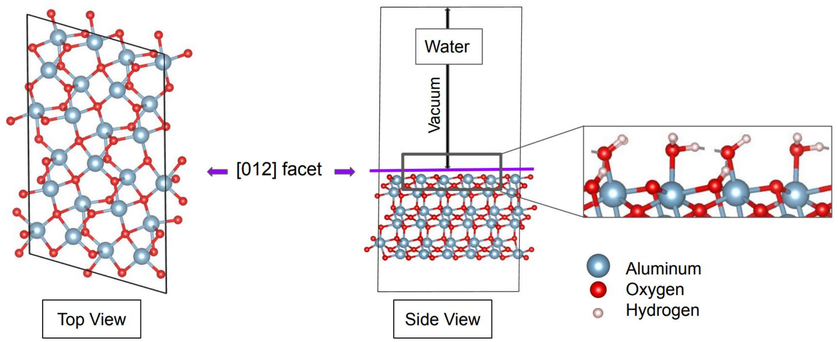
Research Motivation and Background

Selenium, in form of oxo-anions – Selenate and Selenite, has been identified as a toxic substance present in drinking water. Researchers have found that metal oxides nanoparticles such as Hematite and Alumina are the adsorbent materials that can reduce selenium content by adsorbing Selenate and Selenite. The adsorbance capacity depends on many factors including configurations of oxo-anions, the degrees of protonation, and the effect of different adsorbent materials. The goal of this research is using first principle calculations to understand these factors, which are important in designing selective models that can improve water resources efficiently using less energy and low cost.

Methods

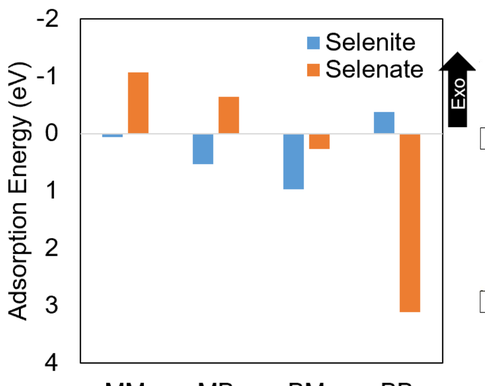
Perform Density Functional Theory using VASP

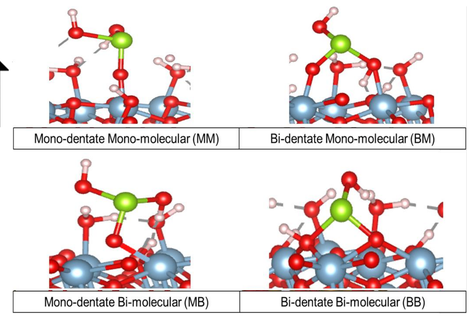


$$E_{adsorption} = E_{Al_2O_3 \cdot (12-y)H_2O \cdot H_2SeO_x} + y\,E_{H_2O} - E_{Al_2O_3 \cdot 12H_2O} - E_{H_2SeO_x}$$

Findings and Progress

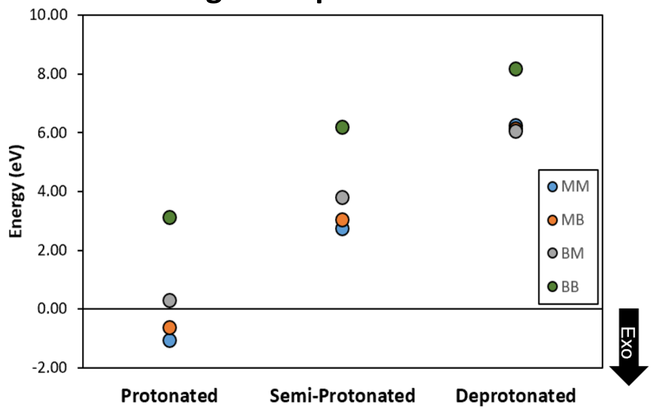
Adsorption of Selenite and Selenate with different configurations on [012] Alumina surface





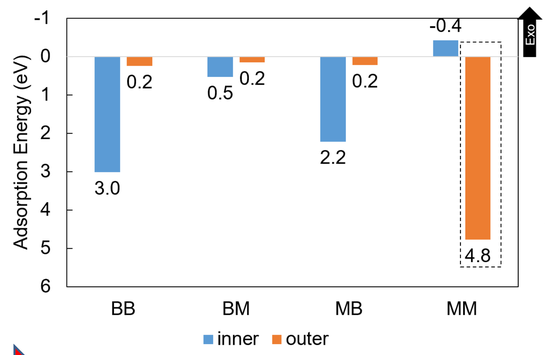
Alumina [012] surface is more selective to selenate adsorption

Adsorption of Selenate on [012] Alumina surface with different degree of protonation



Fully protonated systems have higher adsorption energies

Inner sphere vs. Outer sphere adsorption of selenate on alumina surface



Inner sphere adsorption is stronger than outer sphere adsorption

Conclusions

- Alumina [012] surface adsorption is more selective towards selenate as compared to selenite
- Fully protonated systems have higher adsorption energies than semi-protonated and deprotonated systems
- Inner sphere adsorption is more exothermic than outer sphere adsorption

Acknowledgements

- Dr. Christopher Muhich
- Srishti Gupta
- Muhich Research Team

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