Today Im gonna talk about my research project ~Title

Background: Disinfection byproducts are commonly produced by wastewater treatment methods, specifically halogenated methanes and trihalomethanes are most prevalent.

These can include known carcinogens, such as DCM and chloroform.

The current solution is to use activated carbon, but this has not been studied very well.

The purpose of this study is to study the interactions between the halomethanes and the graphenic surface.

We used circumcoronene as the graphenic model.

It's large enough for the small scale interactions but small enough to not be computationally intensive.

We investigated all possible chloro, bromo, and iodo compounds, included mixed compounds.

We used 40 randomized starting conformers and eliminated them based on Boltzmann distribution and conformation weights

We used a continuum solvation model to simulate an aqueous environment and all the energies were compared to the adsorption of methane

The delta G values were found using this equation and the delta delta G was found by subtracting the adsorption of plain methane from the compound, for each compound

So, here are the series for the single-identity halogen compounds sorted by decreasing halogen content

Chlorine's slope is linear ignoring the nonpolar carbon tet

Bromine has a large jump then increases

Iodine is the only one with a negative delta delta G which makes sense due to the strong dispersive force.

This was all done using Gaussian 16. Optimizations and frequencies were performed using M06-2X/Def2-SCP, and energies were done with Def2-TZVPP.

Looking at the mixed series, I grouped them by total halogens in the compound.

It's not as simple as that, there are some differences based on the identity of the halogens involved.

Overall, the trihalomethanes did have lower energy and included some negative values, which include iodine

Keeping in mind based on the definition of delta delta G, a negative value is a stronger interaction

The strongest interacting compounds were iodine-containing, and the least adsorbing compounds were chloroform and DCM, which were the most important due to their known health effects.

The larger nonpolar compounds demonstrated stronger adsorption in this aqueous context, which makes sense as the more polar compounds would have stronger interactions with the water solvent than the surface

This is far from over, working to develop more trends with the delta delta G based on the identity of the halogen like the chloromethane series or the mixed halogen series.

Also, we're looking at using dipole energy as a way of quantifying that information and also investigating critical points between the surface.

I'd like to thank the EIU Department of Chemistry and Biochemistry for their support in this and also my research advisor Dr. Steven Pellizzeri.

I'd also like to acknowledge the Keiter Summer Fellowship Award, without it, a lot of this work wouldn't have gotten done.

Thank you for listening