Adsorption Energies for Polar Organics Interacting with Clay Minerals. (S11-aggarwal105035-Poster)

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Abstract:

To help understand experimental data in the literature, we used molecular dynamics simulations to estimate the adsorption energies for a series of nitroaromatic compounds interacting with smectite clay minerals. The NPT ensemble was used, and all atoms of the clay, water, and the organics were free to move. Many snapshots from each dynamics trajectory were used to estimate clay-organic interaction energies by computing the difference between the total energy of the system and the energies of the hydrated clay and the organic separately. The algorithm will be presented, as well as the place of these energy calculations in a broader scheme to compute adsorption energies for direct comparison with isotherm data. The results are encouraging in that experimental adsorption maxima for the nitroaromatic compounds correlate fairly well with simulated interaction energies, although some discrepancies were observed. The interaction energy was dominated by electrostatic, rather than van der Waals terms, in accordance with earlier concepts that complexation interactions between interlayer cations and the nitroaromatic molecules are critical. These complexation energies also seem to dwarf the aqueous solvation energies of the nitroaromatics as a contributor to the overall adsorption energy.

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Presentation Information:

Presentation Date: Wednesday, November 13, 2002
Presentation Time: 3:00-5:00 pm

Poster Board Number: 1639

Keywords:
Adsorption energies, Nitro-aromatics, Smectites