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Molecular Dynamics Simulations of Halomethane Adsorption on Two Dissimilar Surfaces GARY LEUTY, CHIRANJIVI LAMSAL, MESFIN TSIGE, Southern Illinois University at Carbondale — In this study, atomic-scale MD simulations were used to study multilayer adsorption of three different halomethane compounds (CF_4, CF_3Cl and CF_3Br) onto two different surfaces (graphite and hydroxylated α-quartz) to show how orientation, layer structure, packing and dynamics vary as a function of temperature and substrate surface characteristics. In this way, non-polar CF_4 on hydroxylated α-quartz is shown to exhibit a highly ordered packing arrangement only weakly dependent on temperature variation. In contrast, interactions between polar adsorbate groups and hydroxyl groups on the surface give CF_3Cl and CF_3Br a very different layer structure at the surface. Analysis of the orientations of polar molecules in the first adsorbed layer shows a lightly ordered arrangement of dipoles, and residence time and dipole correlation calculations suggest that this ordering is subject to frequent shifts in orientation and position within the film.

Gary Leuty
Southern Illinois University at Carbondale

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