

23d Adsorption Behavior of Repulsive Molecules

Timothy E. Wetzel, Gregory L. Aranovich, and Marc D. Donohue

Recently, it has been shown that adsorption of gases on solid surfaces often leads to repulsive forces between adsorbate molecules. In this paper, adsorption of molecules on a one-dimensional lattice is considered for repulsive interactions between adsorbate molecules. Exact adsorption isotherms are calculated and analyzed for finite and infinite chains of active sites (i.e. a one-dimensional lattice). Although the mathematical solution for the one-dimensional lattice is known for attractive and repulsive systems, the effects of intermolecular repulsions on adsorption behavior have not been studied in detail previously. Similarly, while the mathematics for the one-dimensional lattice has been solved for any arbitrary lattice length, the effect of finite size on adsorption isotherms for repulsive adsorbate interactions has never been examined. This paper shows that spatial confinement and strong attraction to active sites can cause compression of an adsorbed phase, and that repulsive interactions between adsorbed molecules result in steps in the adsorption isotherms. For higher chemical potentials, the density increases until saturating at the lattice capacity. These steps in the adsorption isotherm have not been observed in previous studies of lattice systems. For small lattices, the adsorption behavior was found to be fundamentally different for even and odd values of lattice length. Lattices with an even number of lattice sites can have two steps in the adsorption isotherm, whereas systems with an odd number of sites only have a single step occurring at a coverage slightly greater than half the lattice capacity.