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DFT Estimation of Lateral Interactions in Lattice-gas Models of Br and Cl on Ag(100)[1] T. JUWONO, P.A. RIKVOLD, Florida State University — We studied Br and Cl chemisorbed on a Ag(100) surface, using a latice-gas model and the Density Functional Theory (DFT) method. In this model the Br and Cl ions adsorb at the fourfold hollow sites of the Ag(100) surface, which yields a square lattice of adsorption sites. Five different coverages for each kind of adsorbate were calculated. For each adsorbate and coverage, we obtained the minimum-energy configuration, its energy, and its charge distribution. From these data we calculated dipole moments, lateral interaction energies, and binding energies. Our results showed that for Br the lattice-gas model obtained by fitting to the adsorption energies from the DFT calculation is consistent with long-range dipole-dipole lateral interactions using the dipole moments calculated from DFT charge distribution. For Cl we found less consistency, which indicates that long-range dipole-dipole interactions are not sufficient to describe the Chlorine system.

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