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Ab Initio Calculations for Br and Cl adsorption on the Ag(100) surface TJIPTO JUWONO, Florida State University, IBRAHIM ABOU HAMAD, Mississippi State University, PER ARNE RIKVOLD, Florida State University — Ab-initio density-functional methods have been used to find the ground-state configurations of Br and Cl adsorbates on Ag(100) surfaces with coverages of 1/9, 2/9, 1/4, 1/3, and 1/2 monolayers. The supercell slab method was used to calculate the electron-density distributions for each configuration. The charge-transfer function, surface dipole moments, adsorbate resident charge, and adsorption energies were calculated and compared with results from electrochemical adsorption exeperiments and Monte Carlo simulations. The lateral adsorbate-adsorbate interactions and the binding energies were extracted from the adsorption energies using a lattice-gas model. The calculated quantities are weakly dependent on the coverage, and the overall shape of the charge-transfer function is nearly coverage independent.

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