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DFT study of Br and Cl Electrodeposition on Ag(100) 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 lowest energies of Br and Cl adsorbates on Ag(100) surfaces with coverages of 1/9, 2/9, 1/3, and 1/2. The supercell slab method was used to calculate the electron density distributions for each configuration. The electron transfer function, surface dipole moments, adsorbate resident charge, and lateral interaction energies were calculated and compared with results from electrochemical adsorption exeperiments. The calculated quantities are weakly dependent on the coverage, and the overall shape of electron transfer function is nearly coverage independent. The calculations also show electron sharing between neighbouring Br atoms at 2/9 coverage, reminescent of Br_2 molecules. This effect is much weaker or absent for Cl.

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