Monte Carlo Simulations and Experiments for the Electrosorption of Cl and Br on Ag(100)

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We present equilibrium Monte Carlo simulations and chronocoulometry experiments for the electrosorption of Br and Cl on Ag(100) single-crystal electrode surfaces. Two different methods are used to calculate the long-range part of the adsorbate-adsorbate interactions. The first method is a truncated-sum approach, while the second is a mean-field-enhanced truncated-sum approach. To compare the two methods, the resulting isotherms are fit to experimental adsorption isotherms, assuming both a constant electrosorption valency γ and also a coverage-dependent γ. While a constant γ fits the Br/Ag(100) well, a coverage-dependent or potential-dependent γ is needed for Cl/Ag(100).