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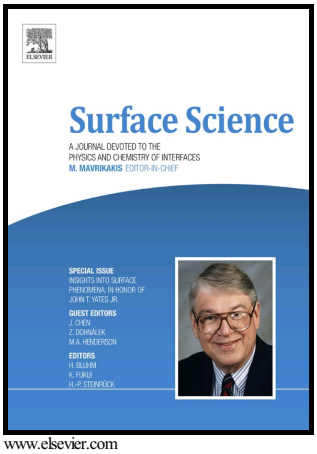

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Abstract

This paper describes the study of a redox species electrosorption on a modified electrode by experimental measurements and computer simulation. The propose model is based on the fact that charges are transferred to the electrode when an electroactive species is adsorbed on its surface. The electrode surface is modified by the irreversible adsorption of a non-electroactive species, which blocks a percentage of the adsorption sites. Hence, the electroactive species can only be adsorbed on the surface vacancies, and, when this phenomenon occurs, interact laterally with the non-electroactive one. Lattice-gas models and Monte Carlo simulations in the Gran Canonical Ensemble are used. The analysis conducted is based on the study of adsorption isotherms and voltammograms, for several values of energies and adsorption degrees of the non-electroactive species. In the case of experimental measurements, an artificial clay (Laponite®) represents the non-electroactive species while the redox probe $Fe(CN)_6^{4-}$ is the electroactive one. The results obtained by the proposed model are compared with experimental voltammograms.

Keyword: Monte Carlo simulation; lattice-gas model; modified electrode surface; redox species; experimental voltammograms, electrosorption.