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Kinetic Monte Carlo applied to the electrochemical study of the Li-ion Graphite System

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Abstract

To delve deeper into the kinetics involved in the staging phenomena of lithium insertion into graphite, it is necessary to develop theoretical models that emulate the physical phenomenon involved. In the present work kinetic Monte Carlo simulations are used to carry out a thorough analysis of the Li-ion graphite system, with the twofold aim of providing atomistic support for interpretations based on several experimental electrochemical techniques commonly used in the laboratory and of making theoretical predictions for future experimental work. Cyclic voltammograms and chronoamperometric transients are obtained, and diffusion coefficients and exchange current densities are calculated at different Li loadings of graphite. These results are compared with selected experimental data from the literature. In this way, there emerge details that cannot be observed in ordinary experiments due to methodological/instrumental limitations. For example, it is found that chronoamperometric responses are different for intercalation and deintercalation, the latter being a faster process. The reason why these phenomena are different is revealed, supporting and widening experimental assumptions. The present results also suggest that