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Simulation of electric double-layer capacitors: evaluation of constant potential method ZHENXING WANG, BRIAN LAIRD, University of Kansas, YANG YANG, DAVID OLMSTED, MARK ASTA, University of California, Berkeley — Atomistic simulations can play an important role in understanding electric double-layer capacitors (EDLCs) at a molecular level. In such simulations, typically the electrode surface is modeled using fixed surface charges, which ignores the charge fluctuation induced by local fluctuations in the electrolyte solution. In this work we evaluate an explicit treatment of charges, namely constant potential method (CPM)[1], in which the electrode charges are dynamically updated to maintain constant electrode potential. We employ a model system with a graphite electrode and a $LiClO_4$/acetonitrile electrolyte, examined as a function of electrode potential differences. Using various molecular and macroscopic properties as metrics, we compare CPM simulations on this system to results using fixed surface charges. Specifically, results for predicted capacity, electric potential gradient and solvent density profile are identical between the two methods; However, ion density profiles and solvation structure yield significantly different results.

[1]Reed et al. J. Chem. Phys., **126**, 084704 (2007)

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