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Intercalation of Li Ions into a Graphite Anode Material: Molecular Dynamics Simulations IBRAHIM ABOU HAMAD, HPC^2, Mississippi State University, MARK NOVOTNY, HPC^2 and Departmenet of Physics and Astronomy, Mississippi State University — Large-scale molecular dynamics simulations of the anode half-cell of a lithium-ion battery are presented. The model system is composed of an anode represented by a stack of graphite sheets, an electrolyte of ethylene carbonate and propylene carbonate molecules, and lithium and hexafluorophosphate ions. The simulations are done in the NVT ensemble and at room temperature. One charging scheme explored is normal charging in which intercalation is enhanced by electric charges on the graphitic sheets. The second charging mechanism has an external applied oscillatory electric field of amplitude A and frequency f. The simulations were performed on 2.6 GHz Opteron processors, using 160 processors at a time. Our simulation results show an improvement in the intercalation time of the lithium ions for the second charging mechanism. The dependence of the intercalation time on A and f will be discussed.

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