

Abstract Submitted
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Anode-electrolyte double-layer of Li-ion batteries: Structure and Li-ion intercalation¹ DAVID O. WIPF, Department of Chemistry, Mississippi State University, IBRAHIM ABOU HAMAD, PER ARNE RIKVOLD, Department of Physics, Florida State University, MARK A. NOVOTNY, Department of Physics & Astronomy, Mississippi State University — The electrochemical double-layer structure plays an important role in Li-ion intercalation during charging of Li-ion batteries with a graphite anode. In our recent Molecular Dynamics studies of a proposed accelerated charging method [I. Abou Hamad *et al.*, Phys. Chem. Chem. Phys. **12**, 2740-2743 (2010)], we notice that ethylene carbonate and propylene carbonate molecules of the electrolyte assemble themselves in a preferred orientation at the electrode-electrolyte interface. On the other hand, they are randomly oriented in the bulk electrolyte. We show that the structure of the double layer is affected by the intercalating Li-ion: while the dipole moments of double-layer molecules far from the intercalating Li-ion point toward the graphite sheets of the anode, they point away from the intercalation site close to the intercalating Li-ion. This observation should contribute to a better understanding of the intercalation process.

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