

MAR14-2013-002982

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Li-ion energy storage of two-dimensional “MXene” transition metal carbides¹

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A new class of two-dimensional early transition metal carbides and carbonitrides, the so-called MXenes, has been synthesized by extracting the “A” element from MAX phases. Experiments have demonstrated that MXenes (Ti_2C , V_2C , Nb_2C , Ti_3C_2 ...) are promising anode materials for lithium ion batteries, delivering high storage capacity and good rate performance. However, the mechanism of Li-ion storage on MXene surfaces is not clear, with counterintuitive differences in predicted vs measured capacities, and large differences between exfoliated and delaminated samples. I will discuss how a strong collaboration between theory and a range of experimental characterization methods, including x-ray adsorption spectroscopy and inelastic neutron scattering, is able to provide a including for the highest measured Li capacities.

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¹Supported by the Fluid Interface Reactions, Structures and Transport Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.