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Energy level offsets and space charge layer formation at electrode-electrolyte interfaces: X-ray photoelectron spectroscopy analysis of Li-ion model electrodes

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Abstract

Energy level offsets and related space charge layer formation are crucial for the kinetic properties of functional electric interfaces. In this contribution, we give a concise overview of our results on model Li-ion cathode interfaces with different overlayer phases obtained by surface science methodology using X-ray photoelectron spectroscopy. In particular, we present electronic energy level alignment, space charge layer formation, and Li1s core level binding energy differences at thin film $LiCoO_2$ surfaces covered by thin layers of solid state electrolyte, other ionic compounds and organic solvents. The data suggest a correlation between the binding energy of the Li1s emission and the extent of the space charge layer formation, which can be rationalized using the concept of ionic energy levels. The data also indicate that interface dipole potentials might be relevant for the formation of some of the investigated interfaces, and suggest that large electronic bulk energy level offsets are insufficient indicators for interface stability, as is usually assumed for electrode-electrolyte interfaces.

Keywords

Li-ion battery; electrode-electrolyte interface; photoelectron spectroscopy; surface science; energy level diagram; space charge layer; ionic interface