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Nonequilibrium Thermodynamics of Li-ion Batteries

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ABSTRACT: Li-ion batteries often involve electrode materials, such as iron phosphate and graphite, which separate into Li-rich and Li-poor phases upon intercalation of lithium. In nanoparticles, this bulk thermodynamic relaxation competes with surface electrochemistry, leading to the fundamental question: *What is the reaction rate during a phase transformation?* A consistent answer is provided by a mathematical theory that unifies and extends the Cahn-Hilliard and Allen-Cahn equations for chemical kinetics and charge transfer. The reaction rate depends on concentration gradients, elastic coherency strain, and other thermodynamic non-idealities. The theory predicts some surprising dynamical phenomena, such as suppression of phase separation in nanoparticles and mosaic instability in porous electrodes, which have since been observed experimentally, not only for Li-ion batteries, but also for other chemical systems.

Biography

Martin Z. Bazant is the Edwin G. Roos (1944) Professor of Chemical Engineering and Mathematics at the Massachusetts Institute of Technology. He earned a PhD in condensed matter physics from Harvard University and joined the MIT faculty in Mathematics in 1998, where he has made fundamental contributions to electrochemistry, electrokinetics, and fluid mechanics. In 2009, he joined Chemical Engineering and started an experimental laboratory. He received the Alexander Kuznetsov Prize in Theoretical Electrochemistry in from the International Society of Electrochemistry in 2015. His other honors include the Paris Sciences Chair (ESPCI), Brilliant Ten (Popular Science Magazine), the Winchell Lecture in Materials Science (Purdue), and the Corrsin Lecture in Fluid Dynamics (Johns Hopkins). He serves on the editorial board of *SIAM Journal of Applied Mathematics* and *Scientific Reports* (Nature Publishing Group) and is the Chief Scientific Advisor for Saint Gobain Ceramics and Plastics, Northboro R&D Center.

