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First-principles molecular dynamics simulations of electrochemical reaction s using the ESM method

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It is important to elucidate a microscopic detail of an electrochemical reaction that takes place at the electrode and electrolyte interface to improve the performance of electrochemical energy storage/harvesting devices, such as secondary batteries, capacitors, fuel cells, and photovoltaic cells. Major difficulties for understanding the reaction are how to incorporate and control the bias potential applied to the interface. To solve these difficulties, we have been developing some intuitive methods to simulate the interfacial electrochemical reaction using first-principles molecular dynamics simulations [1-3]. In this talk I will present our methods and show the bias dependent free-energy profile of the desolvation process of a Li-ion battery and other recent results.

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[3] I. Hamada, O. Sugino, N. Bonnet, and M. Otani, Phys. Rev. B 88, 155427 (2013).