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First-principles Simulation of Electrochemical Systems at Fixed Applied Voltage: Vibrational Stark Effect for CO on Platinum Electrodes ISMAILA DABO, ERIC CANCES, YANLI LI, Paris-Est University, NICOLA MARZARI, MIT — Chemisorbed molecules at a fuel-cell electrode are a very sensitive probe of the surrounding electrochemical environment, and one that can be accurately monitored with different spectroscopic techniques. We calculate from first principles the dependence of vibrational frequencies as a function of the electrode voltage (the vibrational Stark effect) for chemisorbed CO molecules, finding excellent agreement with electrochemical spectroscopic experiments and resolving previous controversies. In the process, we develop a comprehensive electrochemical model to study quantum-mechanical systems as a function of the applied voltage.

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