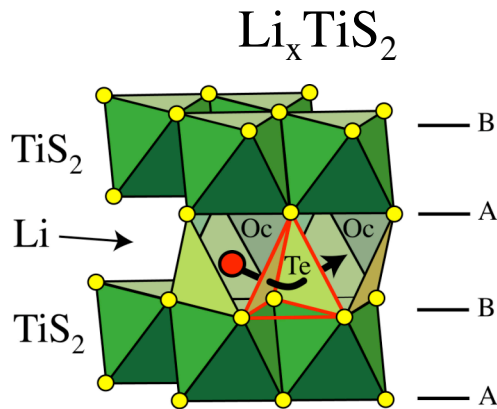
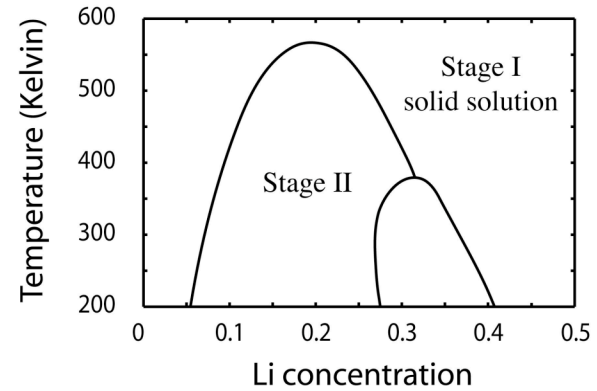


First-principles prediction of diffusion coefficients in Li-intercalation compounds for Li-ion batteries

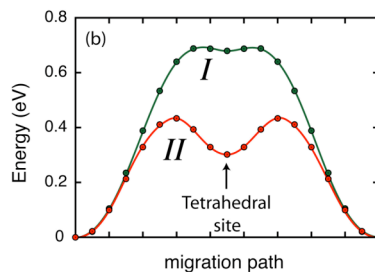
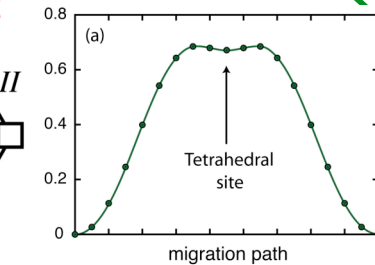
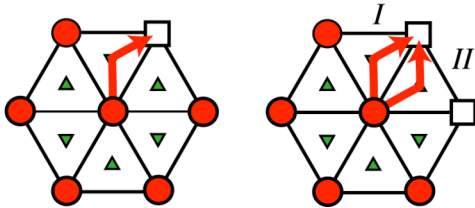


Predicted temperature-composition phase diagram

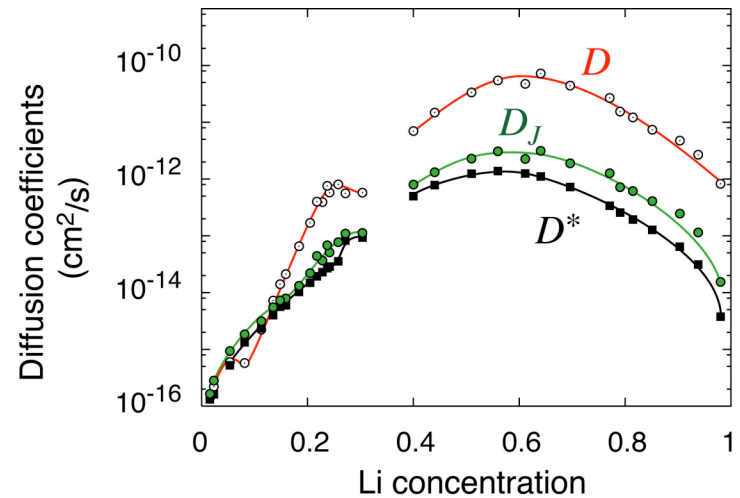


$$J_{\text{Li}} = -D \nabla C_{\text{Li}}$$

Dependence of migration barrier on local environment



Calculated diffusion coefficients as a function of Li concentration



A. Van der Ven, J. C. Thomas, Qingchuan Xu, B. Swoboda, D. Morgan, Physical Review B, 78, 104306 (2008).