SYNOPSYS®

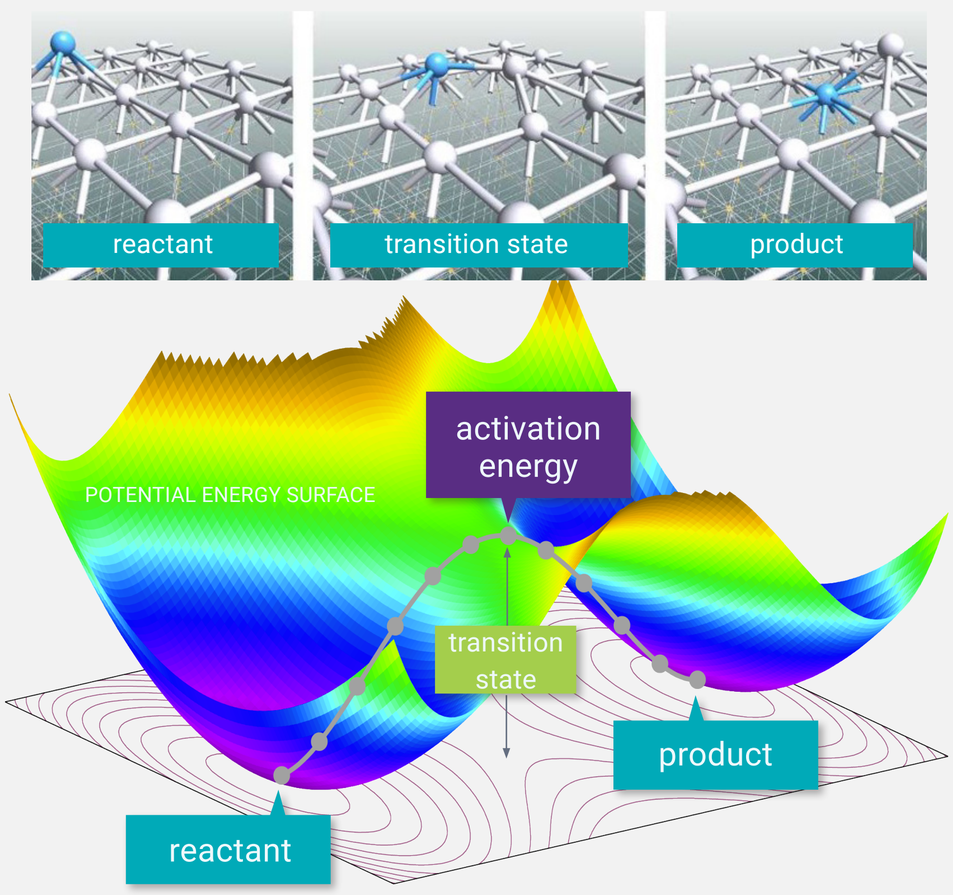
QuantumATK for Atomic-Scale Modeling

Reaction Path Analysis: Battery Applications

Nano-scale simulation package QuantumATK is capable of analyzing a variety of chemical reaction dynamics based on the density functional theory (DFT) and the nudged elastic band (NEB) method.

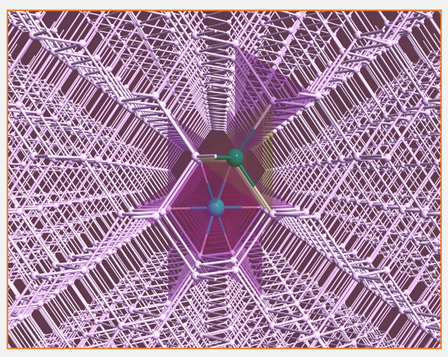
Nudeged Elastic Band (NEB) Method

Find minimum energy paths between two states of a chemical reaction based on DFT and NEB:

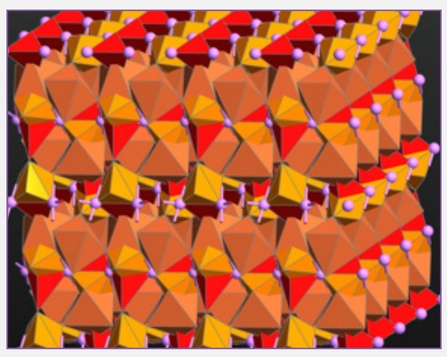


NEB Analysis of Chemical Reactions:

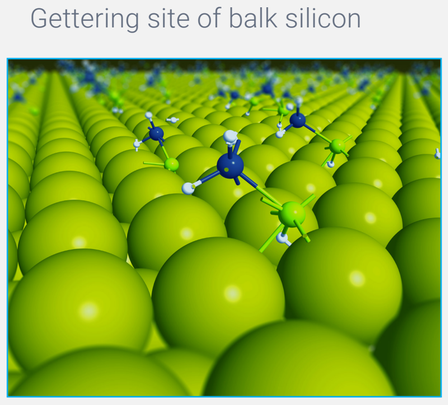
- NanoLab (GUI) helps set up reaction paths in NEB analyses.
- Compute reaction rate constants based on the Harmonic Transition State Theory (HTST).



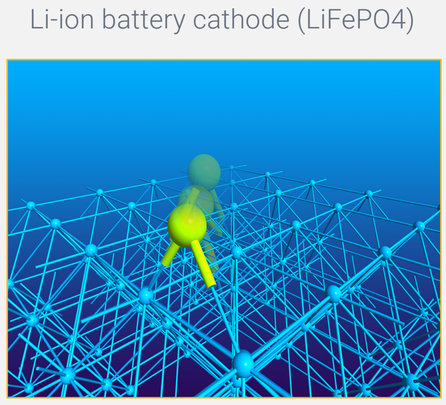
Gettering site of balk silicon



Li-ion battery cathode (LiFePO4)



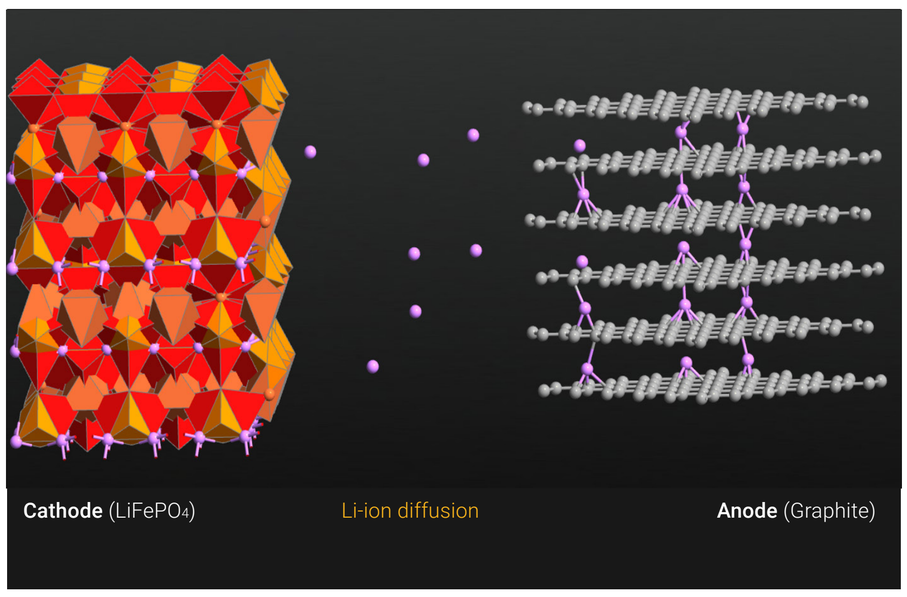
Methanethiol adsorption on an Au surface



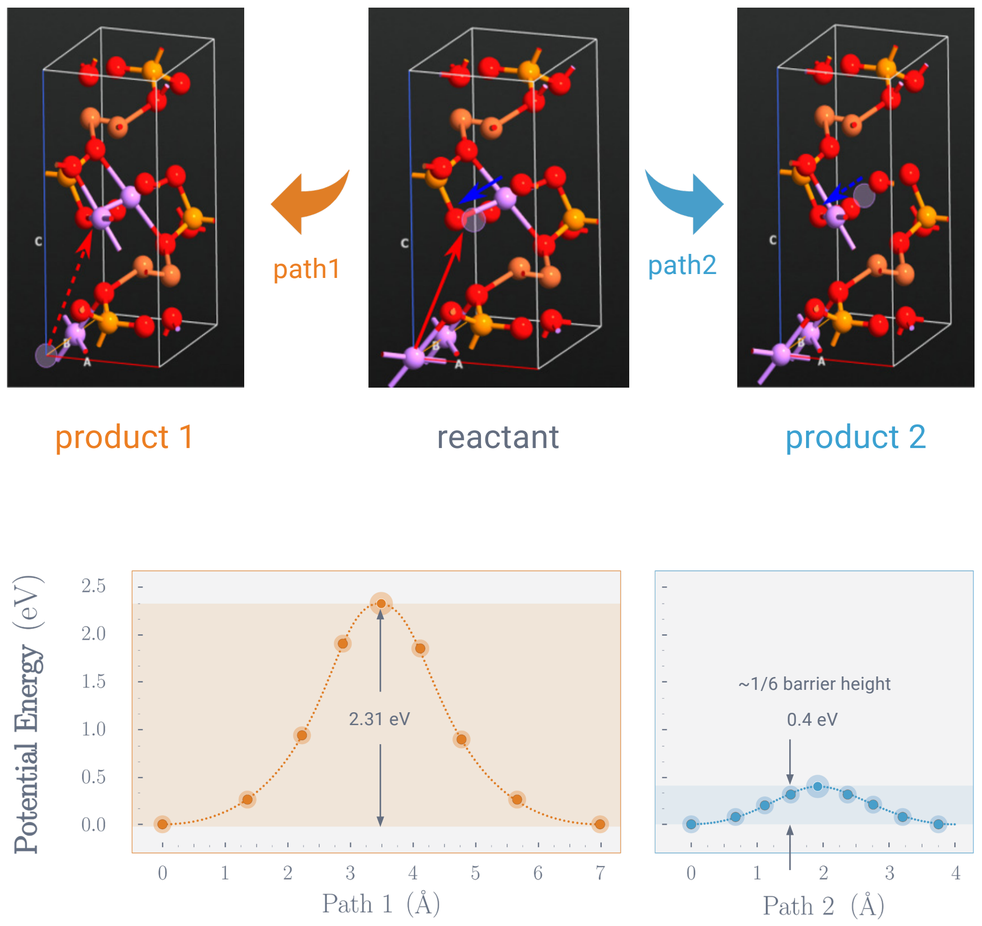
Atomic diffusions on a Pt surface

Simulation: Better Battery Electrodes

NEB-based analysis of Li-ion diffusions in Li-ion battery cathodes ($LiFePO4$)[1]:



Simulation for providing a better cathode structure and alignment where Li ions can easily diffuse.



Align $LiFePO_4$ crystals such that Li ions can easily migrate along the diffusion path 2.

References

[1] M. S. Islam and C. A. J. Fisher, Chem. Soc. Rev., **43**, 185 (2014).