2020 Summer Project at University of Texas, Arlington

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NSF Summer School on Disordered Materials Modeling

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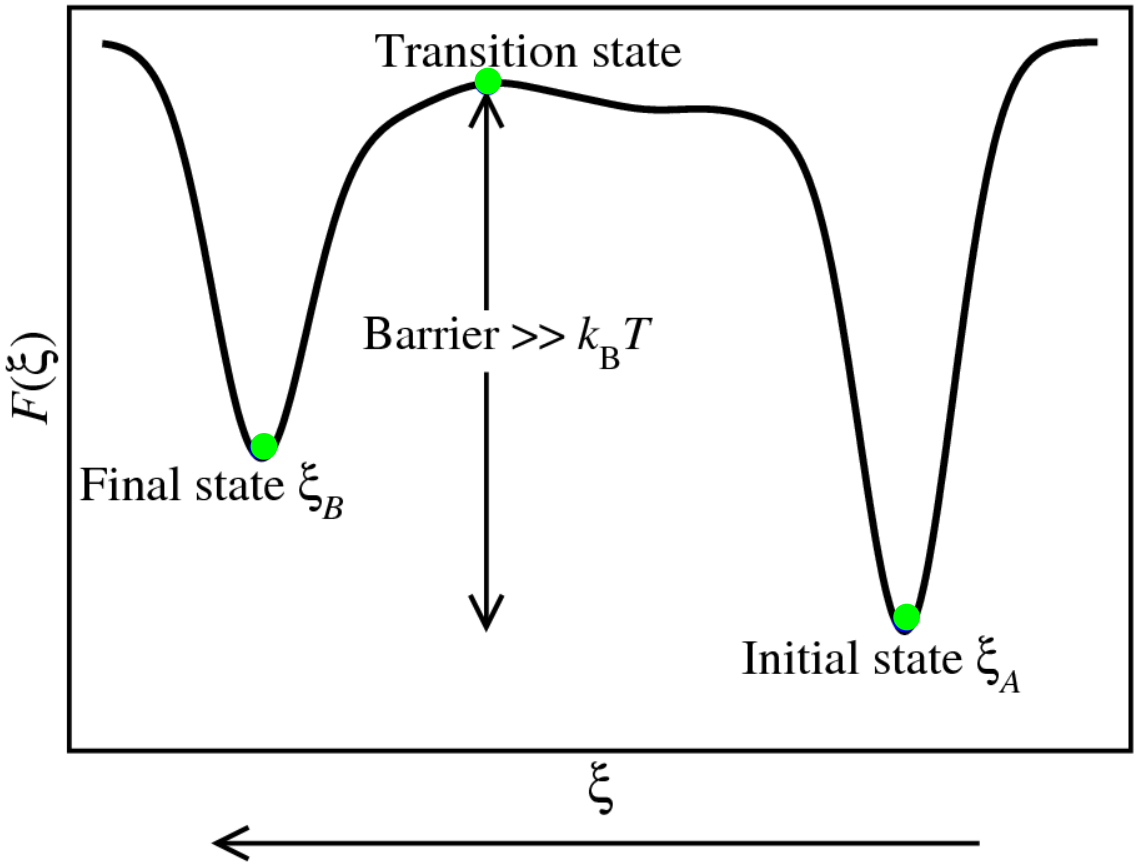
Goal

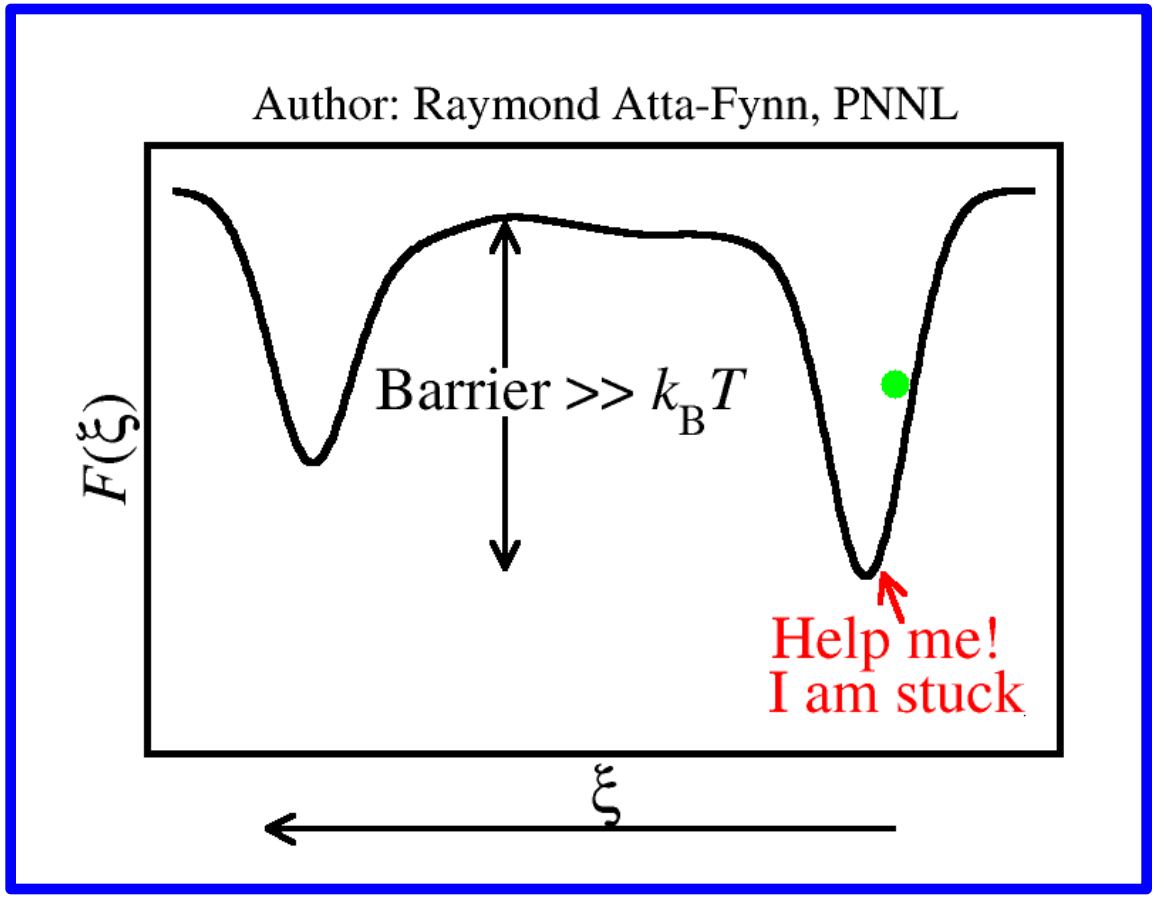
- To use free energy methods for disordered material discovery and simulate reactions in materials

The state of most materials ambient conditions

- Most systems get stuck in state ξ_A at room temperature (300 K)
- The energy barrier must be exceeded for the change from state ξ_A to state the ξ_B to occur.



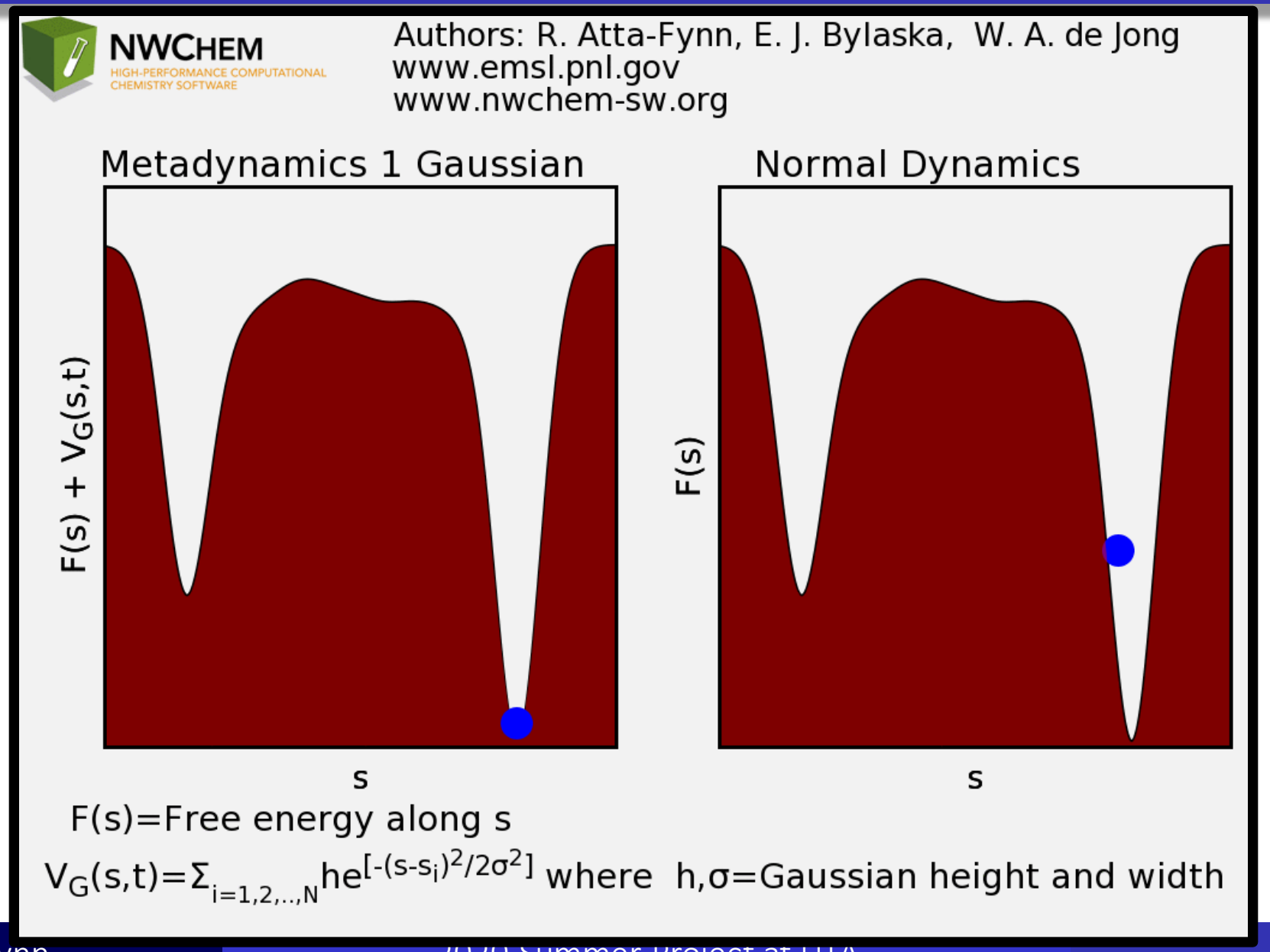
The free energy problem



Use an accelerated rare event sampling technique called metadynamics

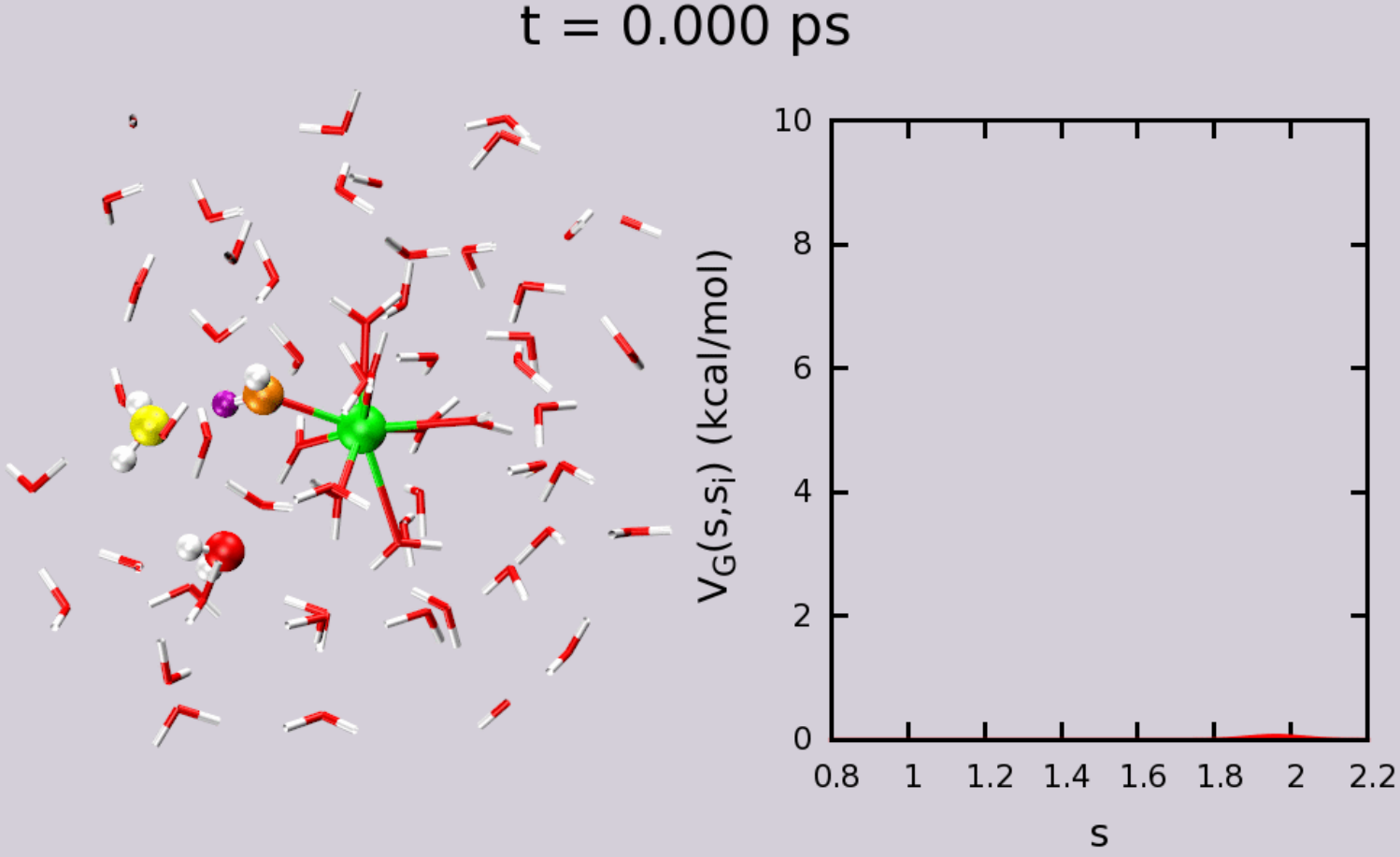
The metadynamics method

- Identify a "good" collective variable **s**
- The system (i.e. atoms, molecule, cluster, or solid) is the "blue ball" in the movie.
- Periodically add external Gaussian bias potentials at the current value of **s** (think of water filling a well to push the ball)
- This system is "forced" to visit new states



The metadynamics method

- One can model all sorts of physical and chemical processes
- Shown here is the metadynamics simulation of the deprotonation reaction of a solvated metal cation.
- The collective variable in this case is the H-O-H bond coordination of O with respect to H.



$U^{4+}(aq)$ ---> $[U(OH)]^{3+}(aq)$ + $H_3O^+(aq)$

Sketch of the 2020 summer project

- Apply metadynamics to search for new configurations of disordered materials using well-chosen collective variables

- Use the metadynamics approach develop a standard protocol to model high-quality atomistic models of disordered materials of varying compositions.