

# Multiscale Modeling of the Mechanical Responses of Solids

## Lecture 2: Time Scales

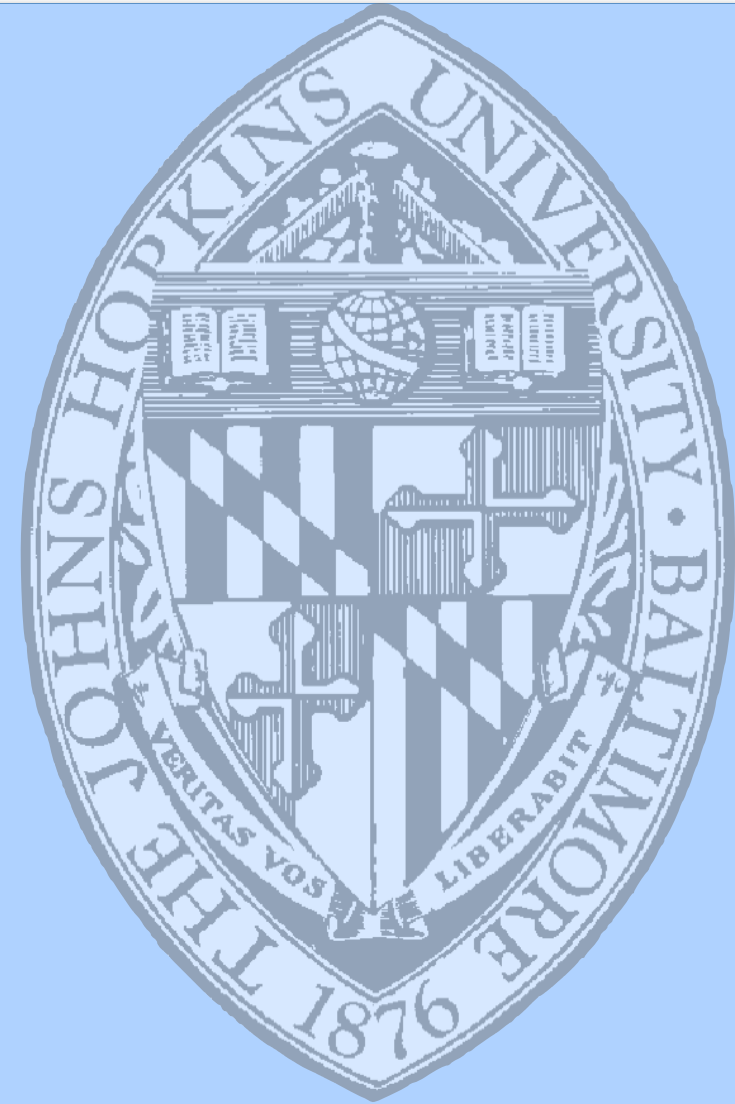
*Michael L. Falk*

*Johns Hopkins University*

*Materials Science and Engineering;*

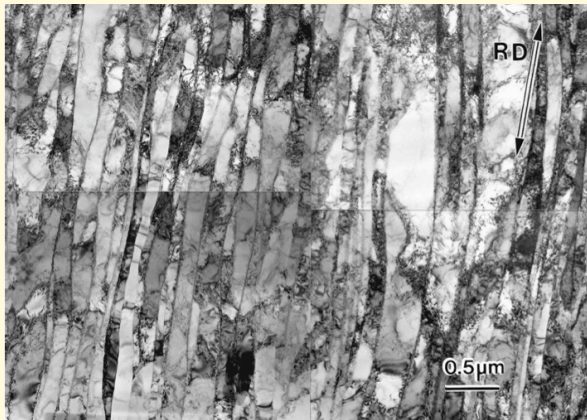
*Mechanical Engineering;*

*Physics and Astronomy*



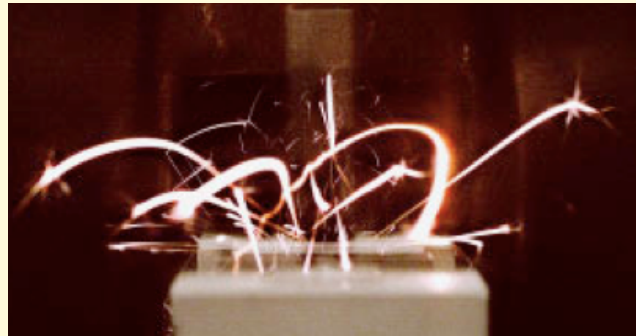
# Materials Processes Far From Equilibrium

- Materials can be driven far from equilibrium due to operating conditions or processing
- Equilibrium theory is of limited utility in predicting behavior of these systems
- Computation can play an important role in these cases



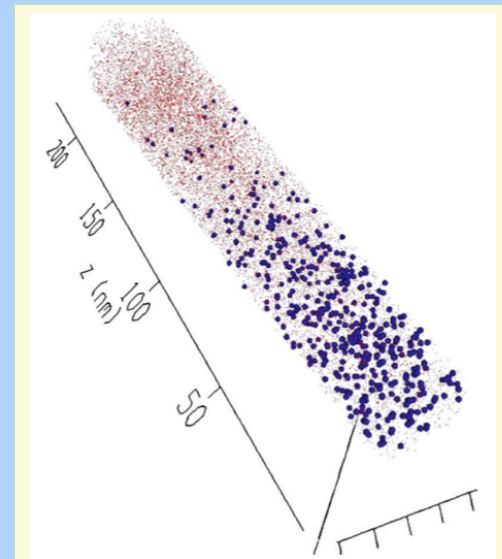
Dislocation patterns in Ni after cold rolling to large strain

From D. Hughes and N. Hansen, *Acta Mat* 48, 2985 (2000).



Sparks during fracture of Zr based bulk metallic glass

C.J. Gilbert, *APL* 74, 3809 (1999).



As dopants in Si revealed by atom probe

From K. Thompson, et al., *APL* 87, 052108 (2005).

# Molecular Dynamics Simulation

- **When time scales are sub-microsecond or behavior is load controlled we can perform molecular dynamics simulation (MD).**

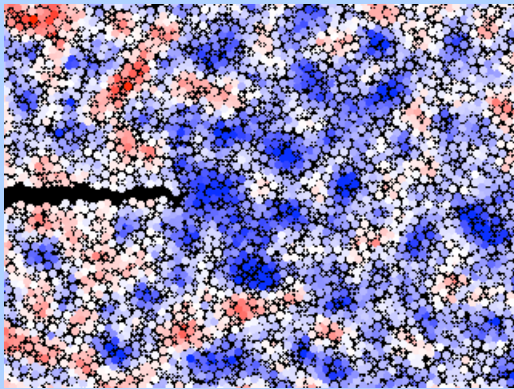
Dynamic fracture in  
polydisperse 2D model of  
a metallic glass,  
MLF, PRB 1999

Sputtering of BN by Xenon ions  
J.T. Yim, MLF, I.D. Boyd,  
JAP 2007

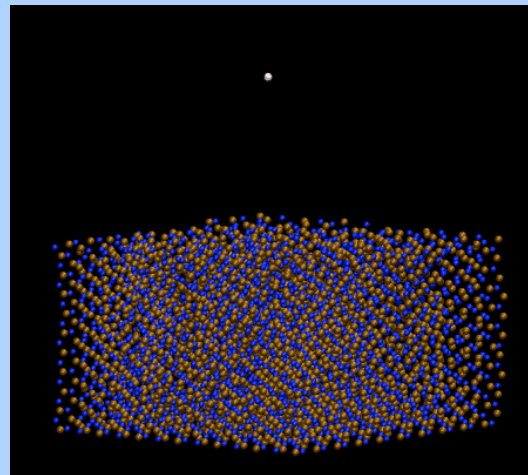
Shear band in metallic  
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Y. Shi, MLF, PRB 2007

# Molecular Dynamics Simulation

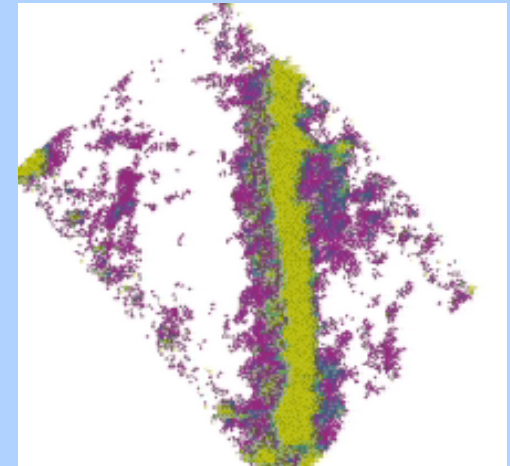
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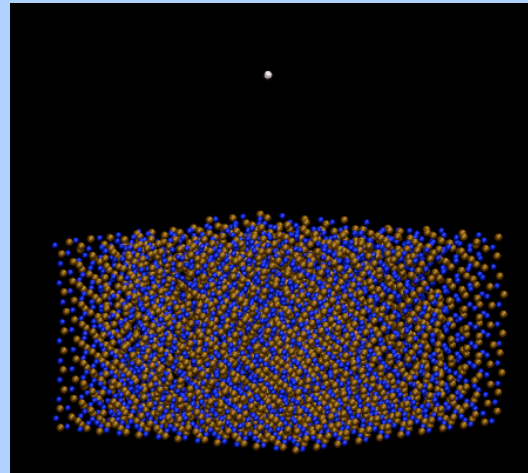
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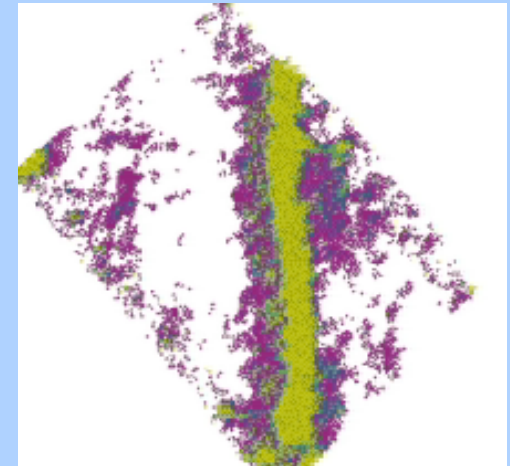
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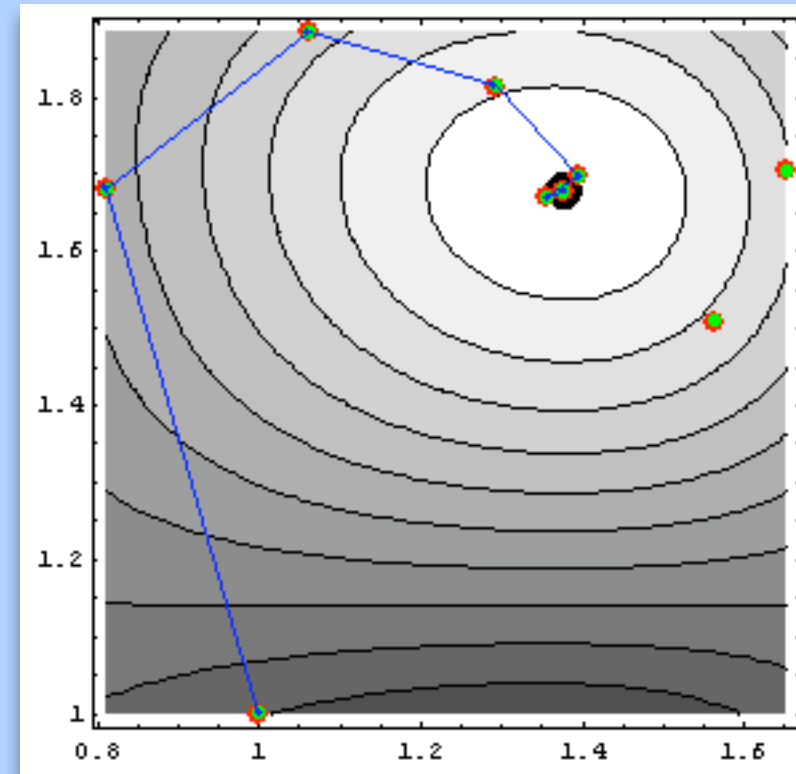
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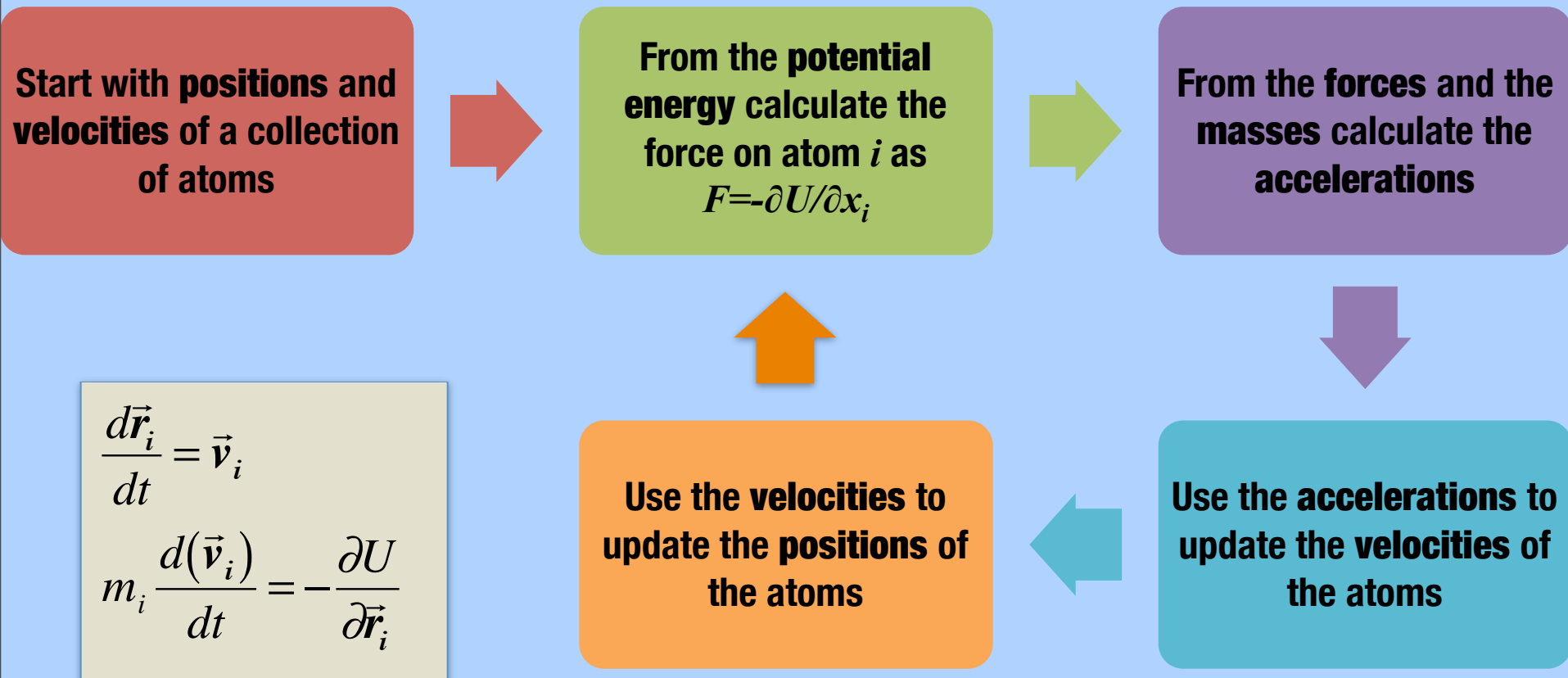
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compression,  
Y. Shi, MLF, PRB 2007

# Limits of Energy Minimization

- **Methods like QC that rely on energy minimization typically cannot include thermally activated processes.**
- **The system is minimized to the nearest local potential energy minimum and cannot escape unless an external load is applied.**
- **This precludes effects of inertia, mass transport and other activated processes.**



# Overview of Molecular Dynamics



# Numerical Implementation

- In order to integrate these equations forward from an initial condition a finite differencing scheme is used
- There the choice of the interval between calculated times is crucial for determining numerical stability
- Too large a time interval results in errors growing out of bound
- The time step must be significantly smaller than the shortest physically relevant process
  - Gas: time for the fastest atom to cross an atomic radius ( $a/v^*$ )
  - Solid: period of vibration for an atom in the presence of its neighbors (inverse of the Einstein frequency)

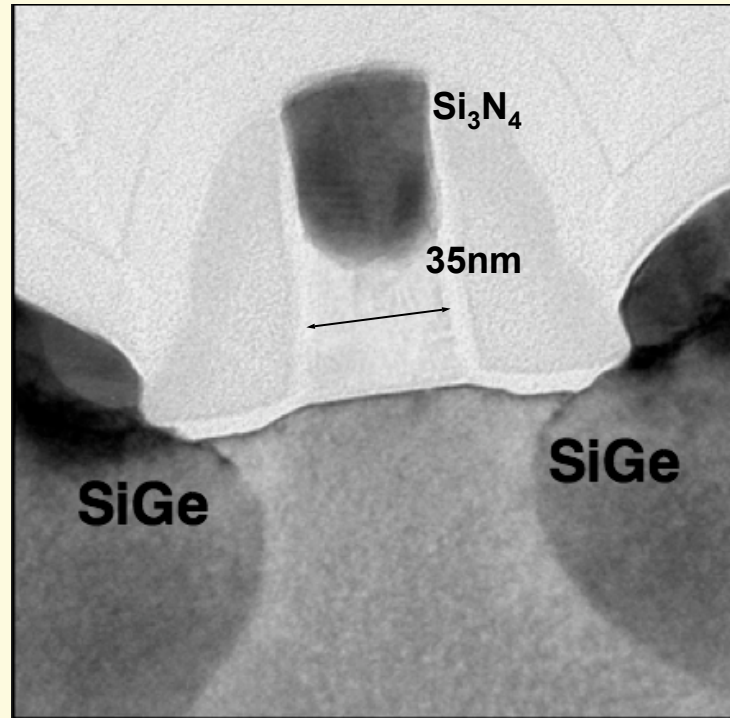


# Limitations of MD

- Because time steps must typically be on the order of 10 fs ( $10^{-14}$  s) in solids, simulations are  $< 1\mu\text{s}$
- Processes that depend on thermally activated rare events are often out of reach of MD
  - Solid-state diffusion and processes limited by SSD
  - Mechanical processes that occur on longer time scales like creep
  - Dissipative processes like frictional sliding
  - Catalysis and other chemical reactions

# Diffusion in Semiconductor Devices

## X-TEM of Intel 35nm PMOS

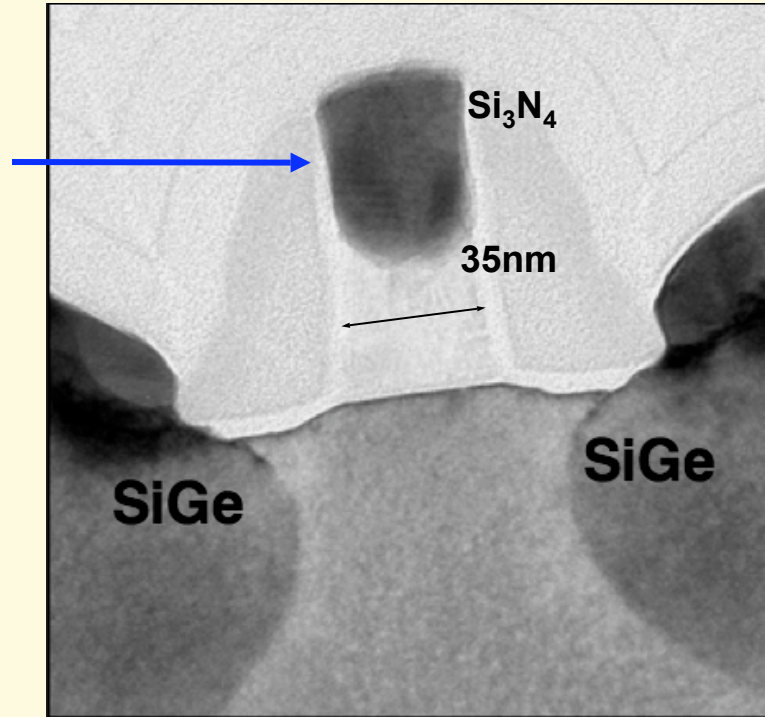


From: S. Tyagi, An Advanced low power, high performance, strained channel 65nm technology, 2005 IEEE International Electron Devices Meeting (IEDM) December 5–7, 2005

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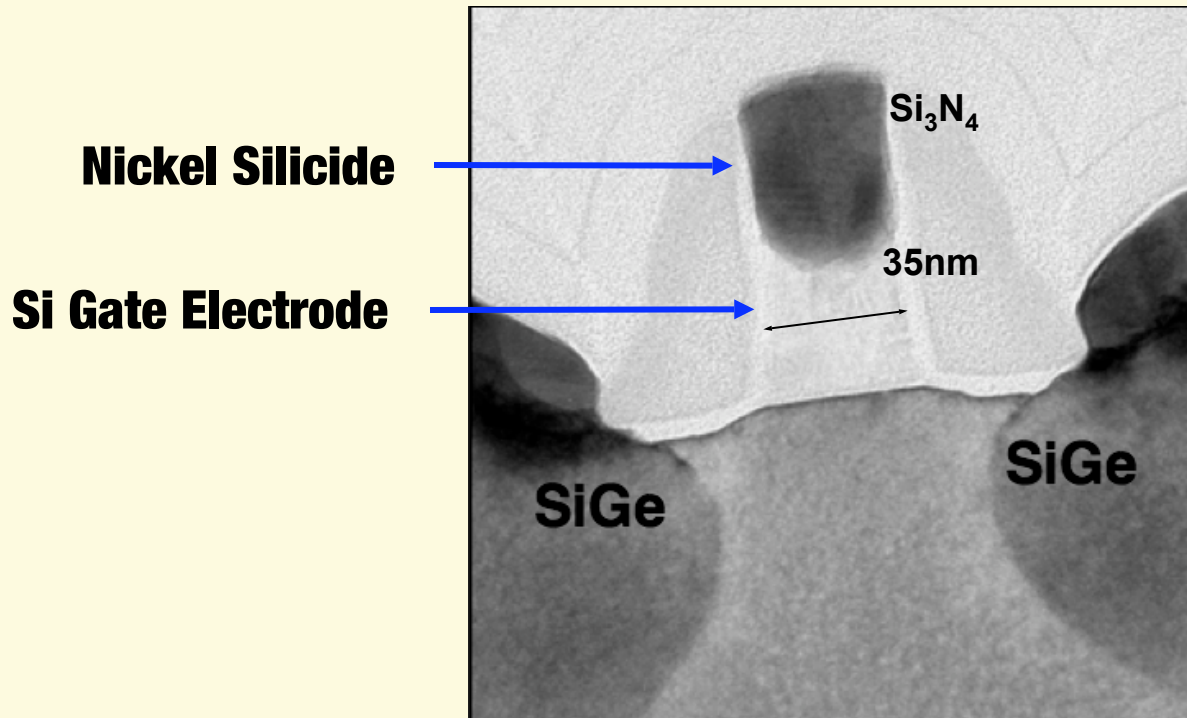
**Nickel Silicide**



From: S. Tyagi, An Advanced low power, high performance, strained channel 65nm technology, 2005 IEEE International Electron Devices Meeting (IEDM) December 5–7, 2005

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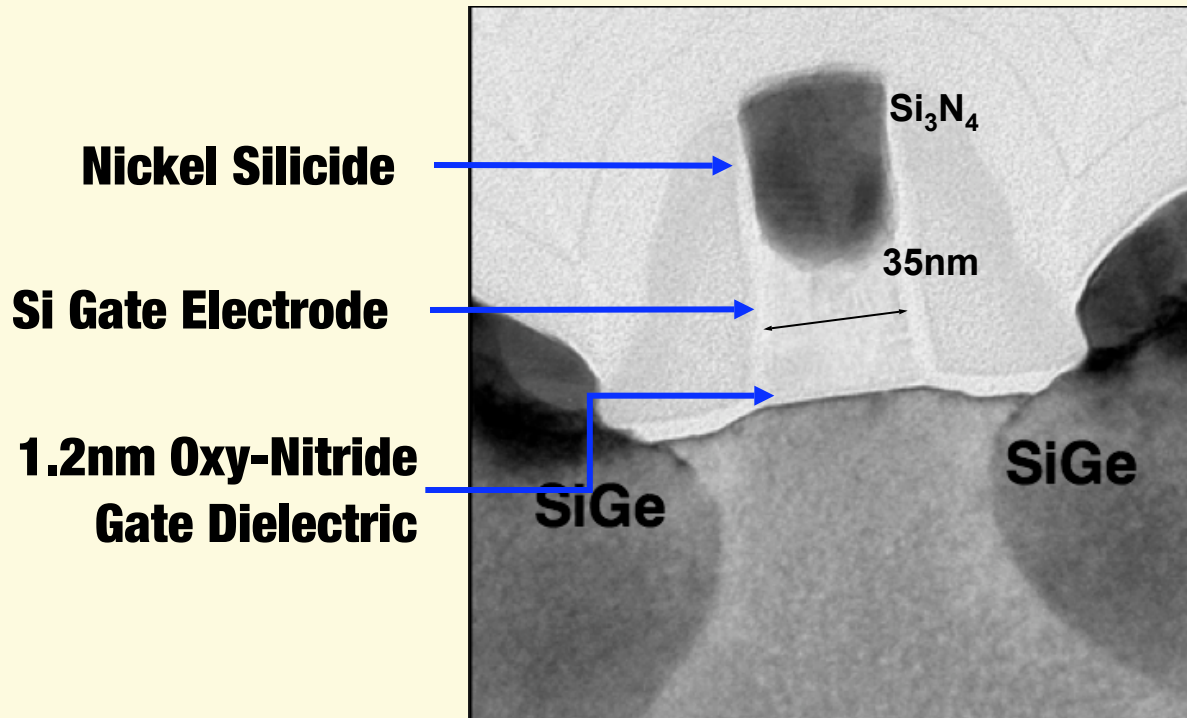
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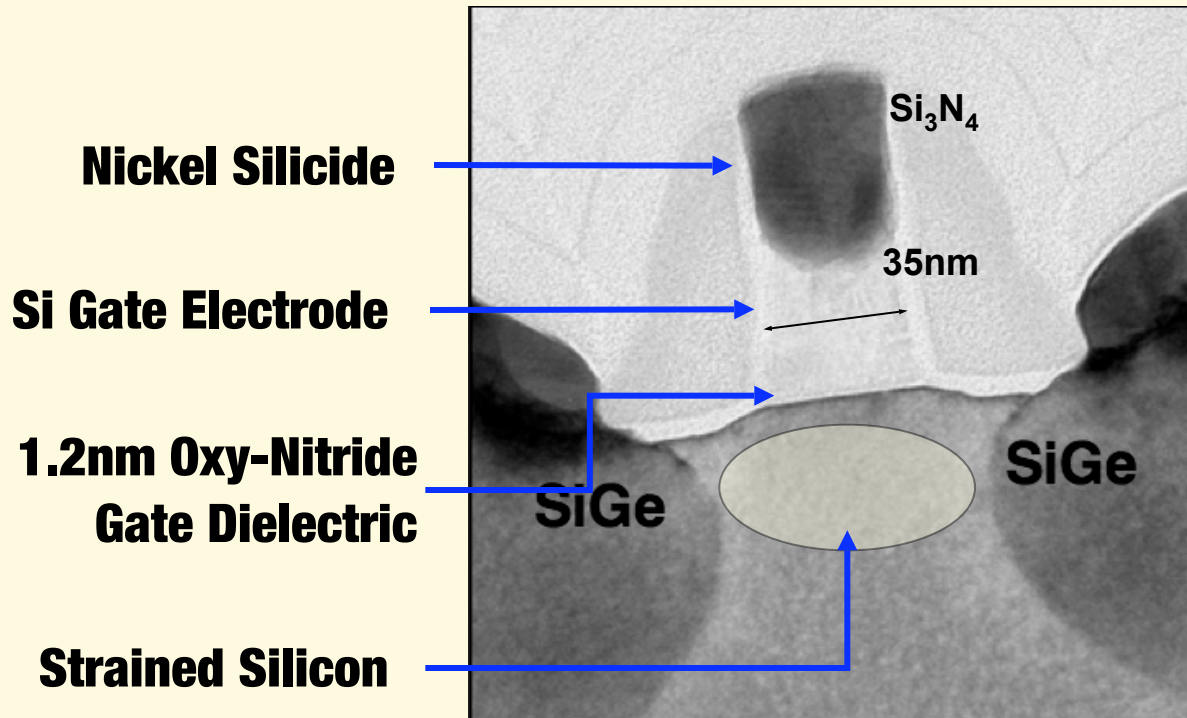
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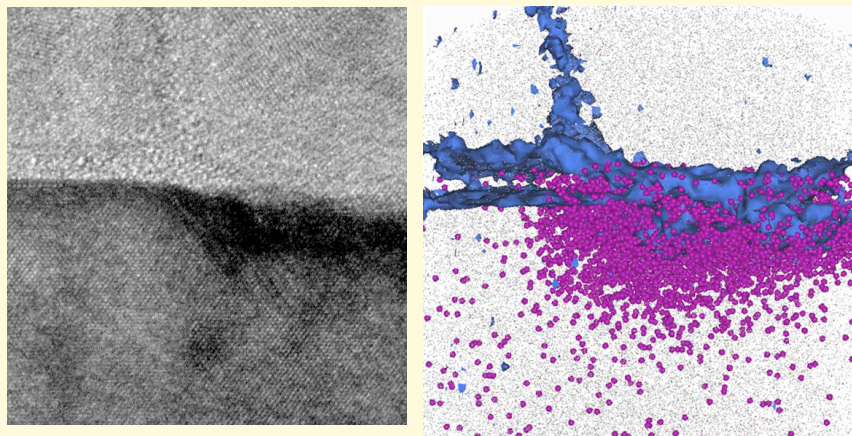
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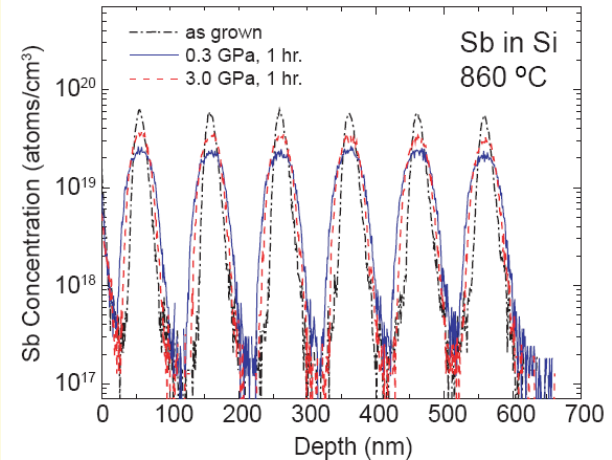
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# Importance of Doping Profiles



TEM image and LEAP 3D reconstruction of a patterned semiconductor test structure. Polysilicon deposited on a  $\langle 100 \rangle$  single crystal silicon wafer. Arsenic dopants shown in purple.

Figure from Imago Scientific Instruments

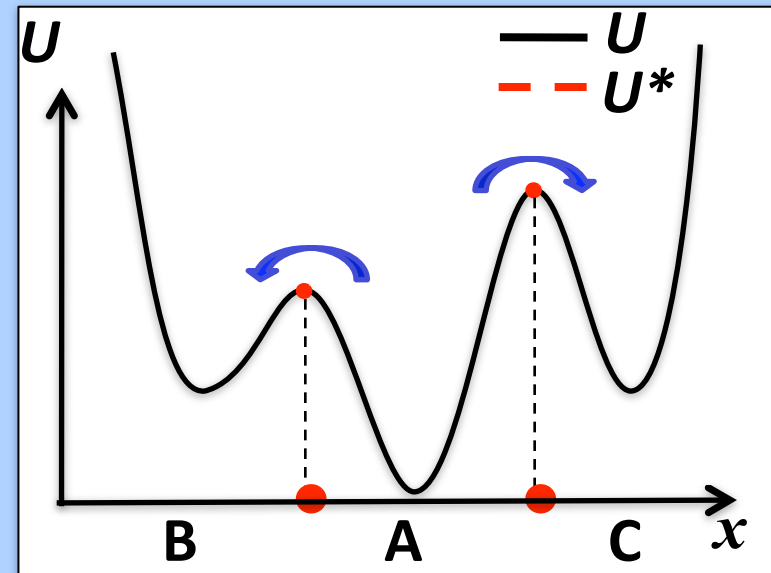
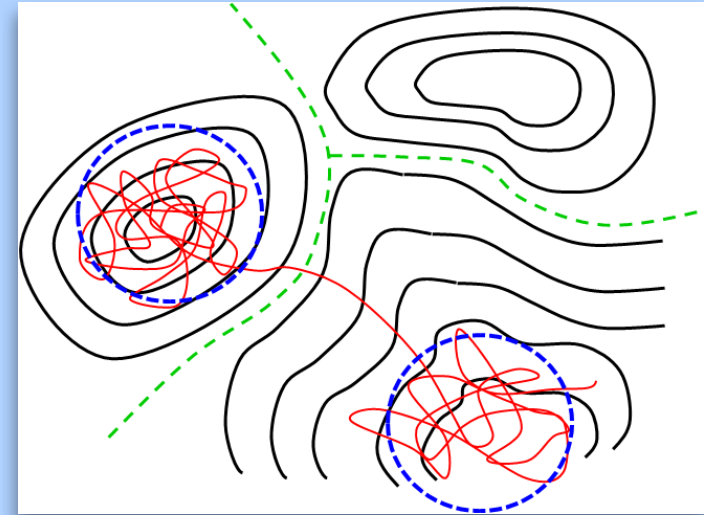


Sb diffusion under hydrostatic compression

Figure from M.J. Aziz, Y. Zhao, H.J. Grossman, S. Mitha, S. P. Smith, D. Schiferl, Phys. Rev. B 73, 054101 (2006).

# Transition State Theory

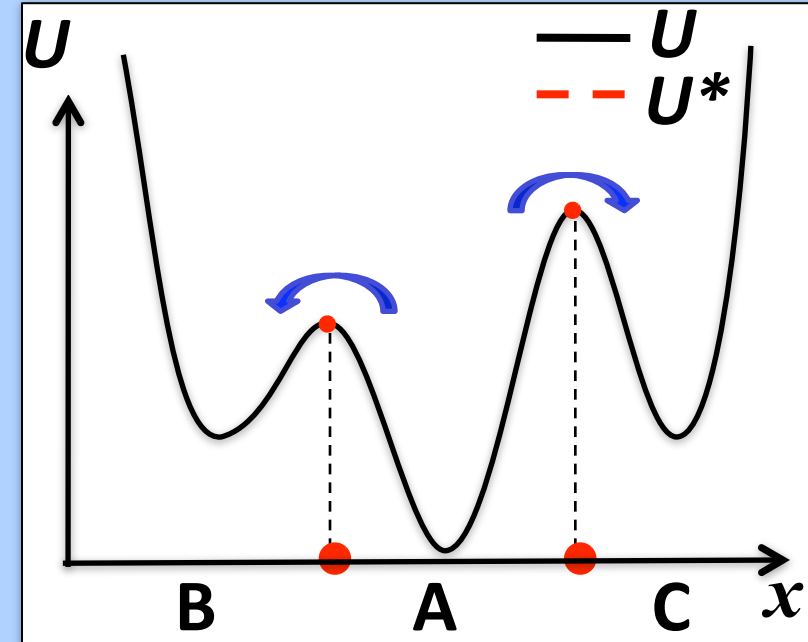
- TST is the fundamental basis of methods discussed today.
- We think in terms of the potential energy landscape.
- This landscape is riddled with potential energy minima (wells).
- Since low energy states are preferred the system spends most of its time vibrating about one or another of these minima.
- Consider cases in which the natural vibrational period within the well is much longer than the transition time.





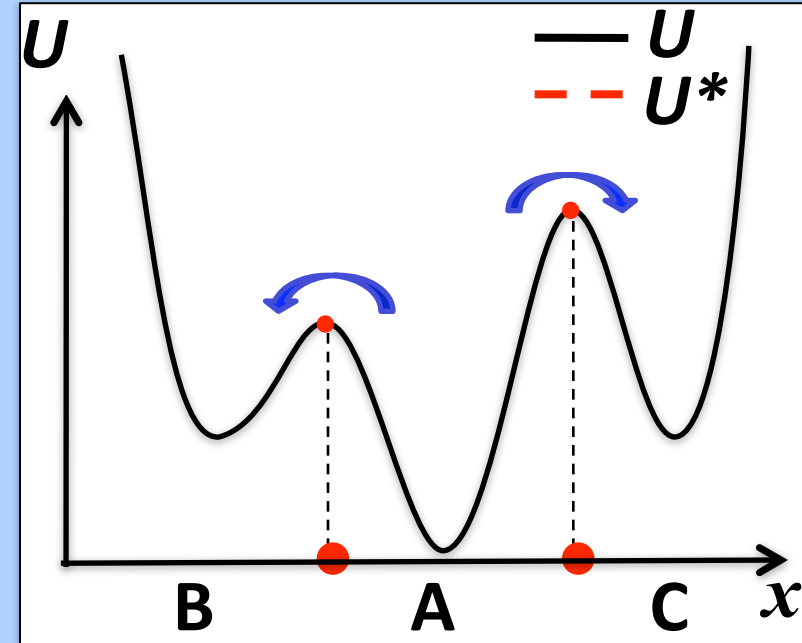
# Transition State Theory

- If this is true, the system has sufficient time to forget how it got into the well it currently occupies (decorrelation), so the escape times must be a Poisson distribution.
- Also the system has sufficient time to fully (ergodically) explore each well before making a transition we can consider transitions using equilibrium statistical mechanics.
- We must define a bounding surface that separates those states inside and outside the well.



# Transition State Theory

- Take the Boltzmann weighted average of the velocity with which the system crosses the dividing surface between A and B
- $\Omega_A$  denotes those points in the basin of attraction of A
- $S_{AB}$  denotes those points on the dividing surface between A and B
- $\Theta(\vec{v} \cdot \hat{n})$  enforces that the average is only over trajectories exiting A.



$$R_{A \rightarrow B} \approx \frac{\int dr^{3N-1} \int_{-\infty}^{\infty} dv^{3N} (\vec{v} \cdot \hat{n}) \Theta(\vec{v} \cdot \hat{n}) \exp\left(-\frac{\frac{1}{2}mv^2 + U(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \int_{-\infty}^{\infty} dv^{3N} \exp\left(-\frac{\frac{1}{2}mv^2 + U(\vec{r})}{k_B T}\right)}$$

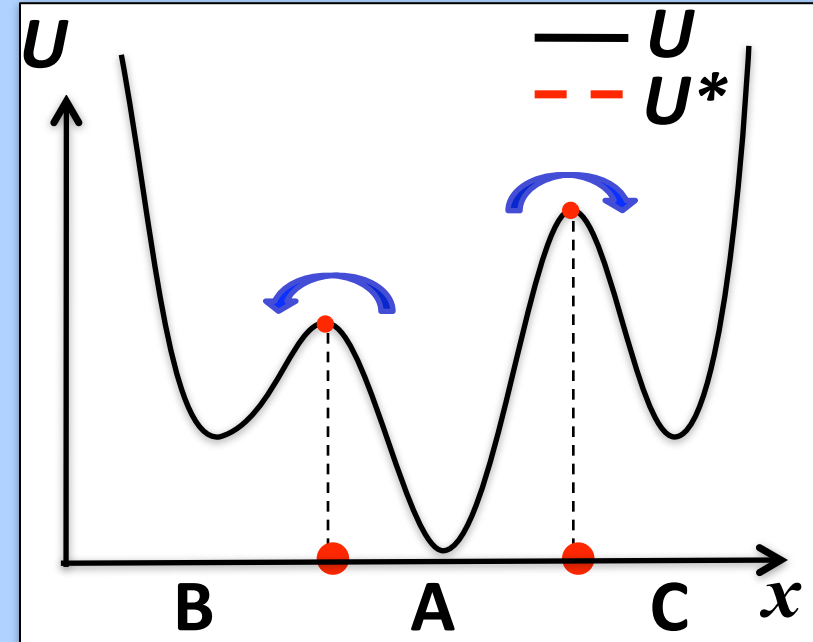
# Harmonic Transition State Theory

- If we assume that the integral can be approximated by a Gaussian, we obtain the well known Arrhenius result

$$R_{A \rightarrow B} \approx f \exp\left(-\frac{U_{AB} - U_A}{k_B T}\right)$$

where  $U_{AB}$  is the energy at the saddle point between A and B.

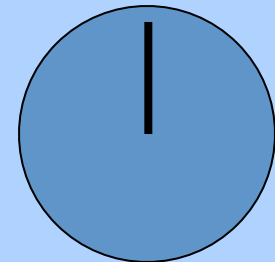
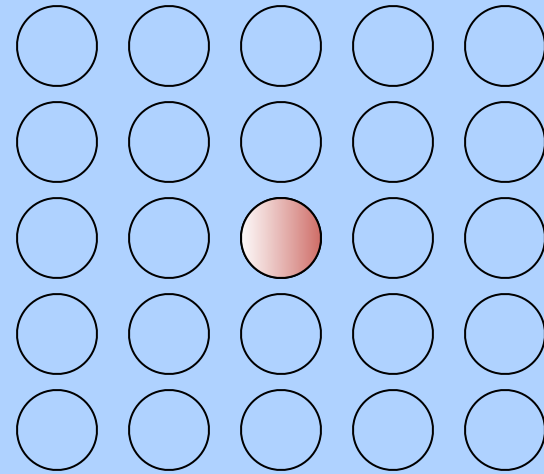
- The “**attempt frequency**”  $f$  can be obtained by dividing the product of the positive eigenvalues of the Hessian at the minimum at A by the product of the positive eigenvalues of the Hessian at the saddle point between A and B



$$f \approx \frac{\det^+ \left[ \frac{\partial^2 U}{\partial r_i \partial r_j} \Big|_A \frac{(m_i + m_j)}{m_i m_j} \right]}{2\pi \det^+ \left[ \frac{\partial^2 U}{\partial r_i \partial r_j} \Big|_{AB} \frac{(m_i + m_j)}{m_i m_j} \right]}$$

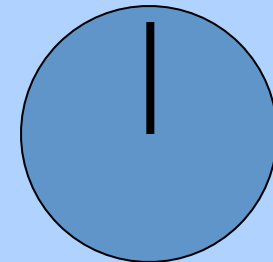
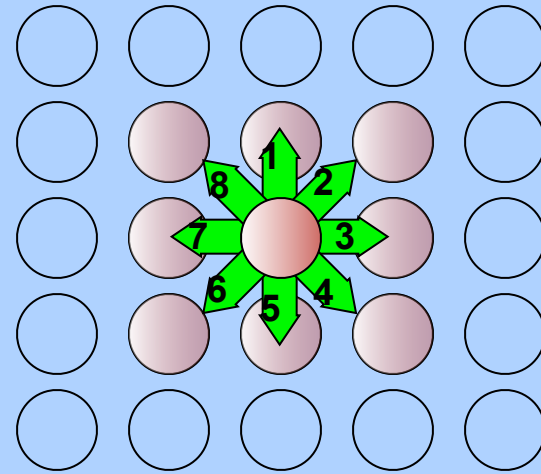
# Kinetic Monte Carlo Simulation

- For stochastic processes like mass transport Kinetic Monte Carlo simulation provides a relatively fast way to take into account atomistic details
  - Start by enumerating all possible transitions and their rates  
 $R \sim f \exp(-E^*/kT)$
  - Select a transition with a probability proportional to its rate.
  - Advance the clock by a time chosen from a Poisson distribution with a time constant given by the net rate of all transitions.



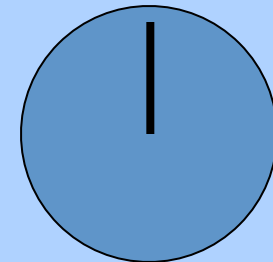
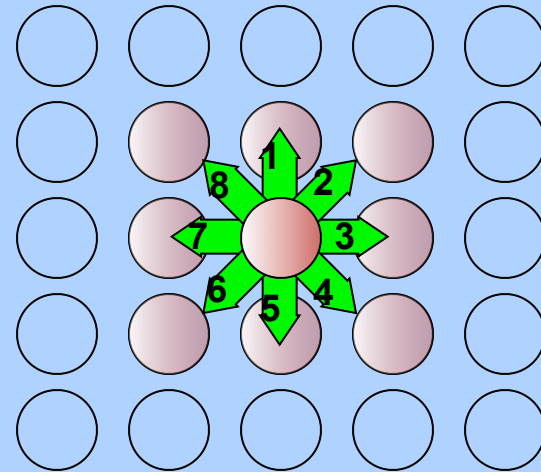
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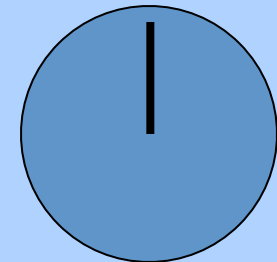
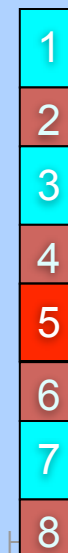
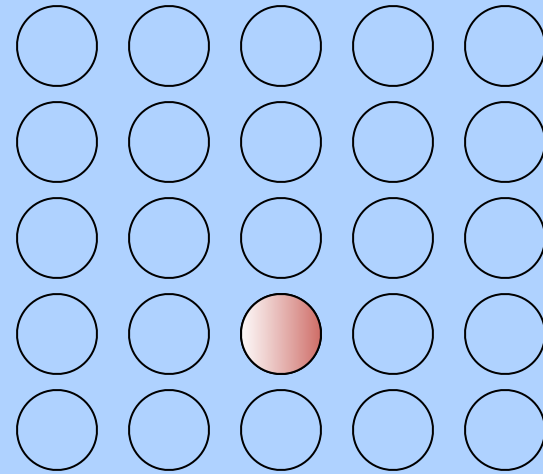
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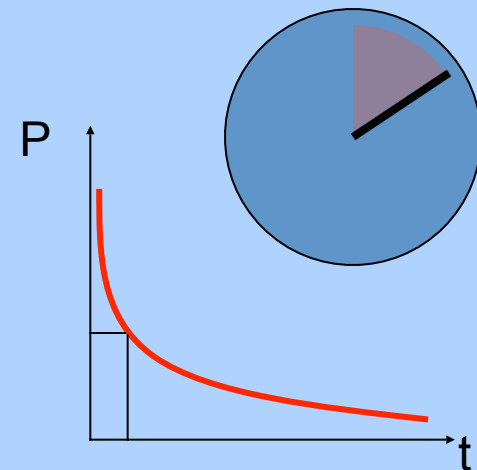
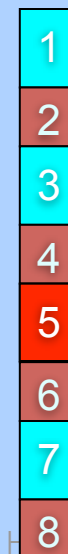
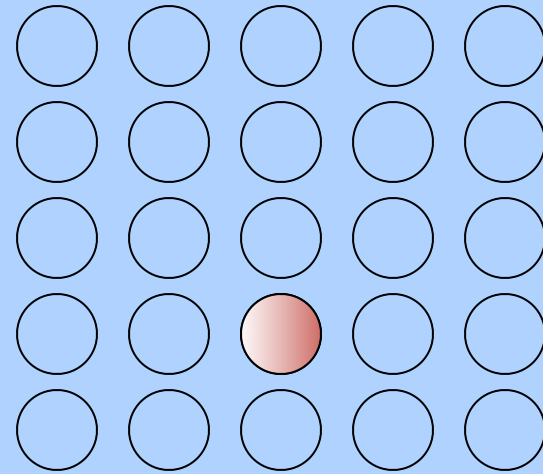
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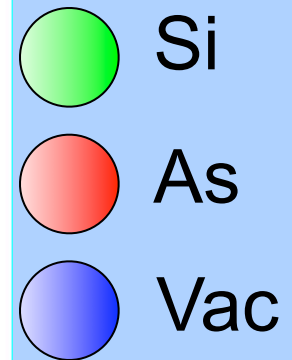
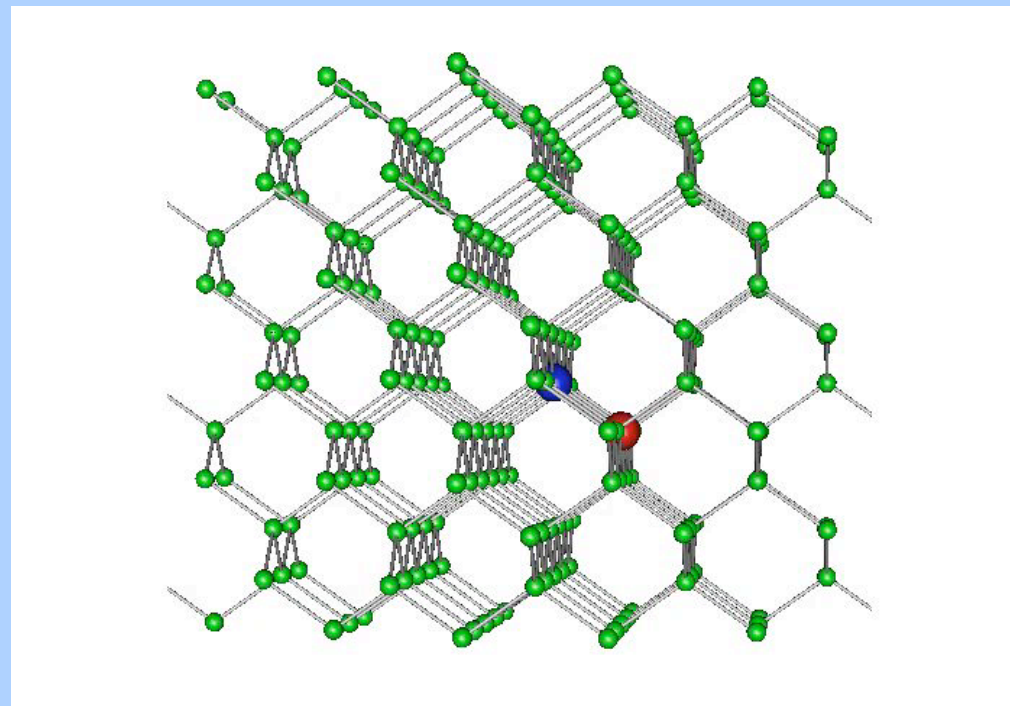
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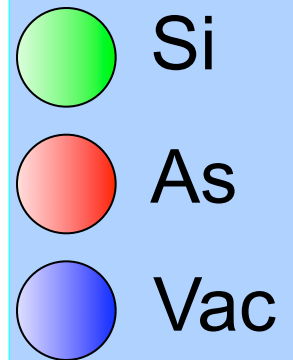
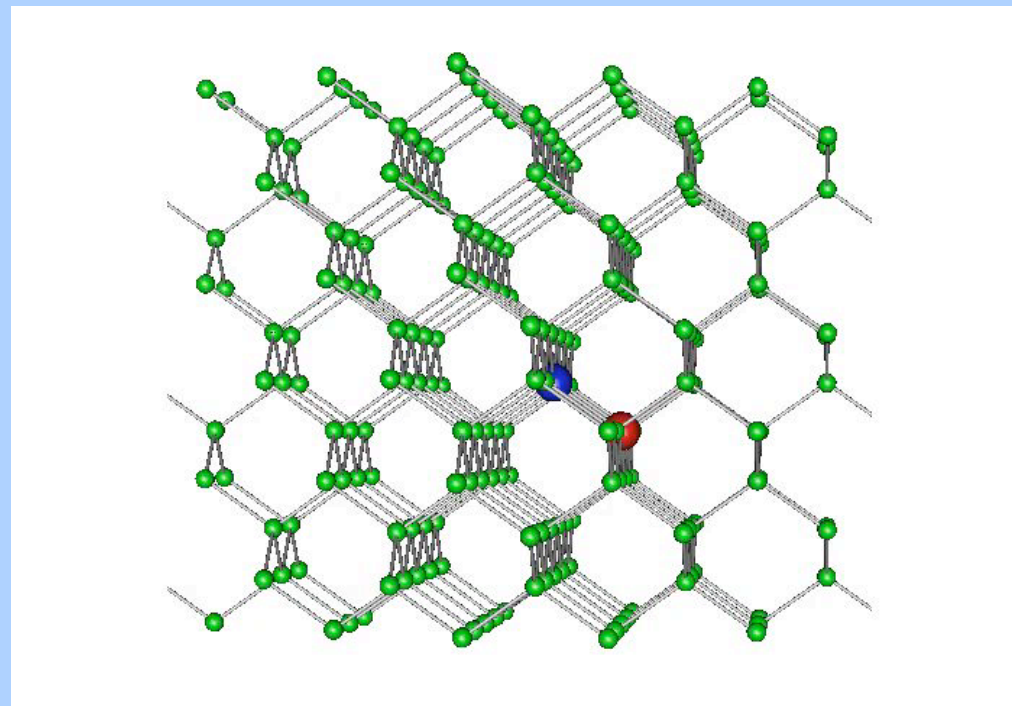
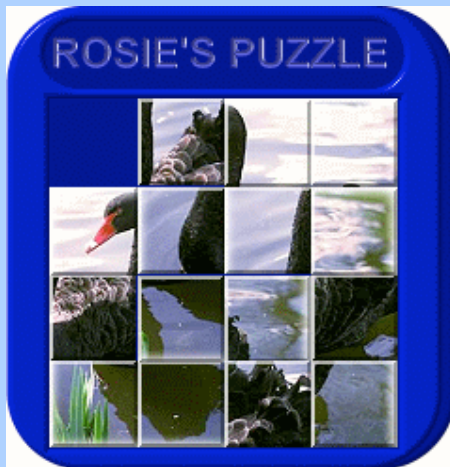
# Simulation of Activated Complexes

- Dopants do not typically diffuse via an exchange mechanism
- Like moving a single colored square in a penny puzzle, the motion of the missing piece, the vacancy, is crucial
- Diffusion of a dopant require a complex coordinated interaction with a mobile defect: either a vacancy or interstitial



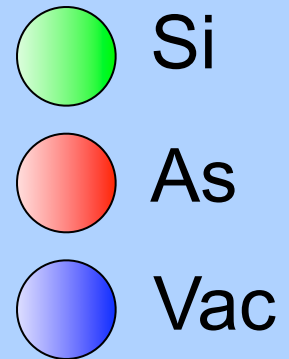
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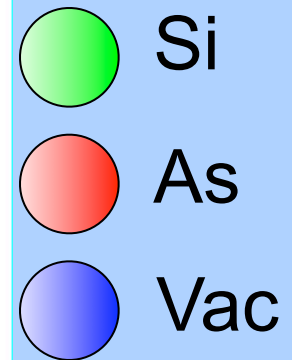
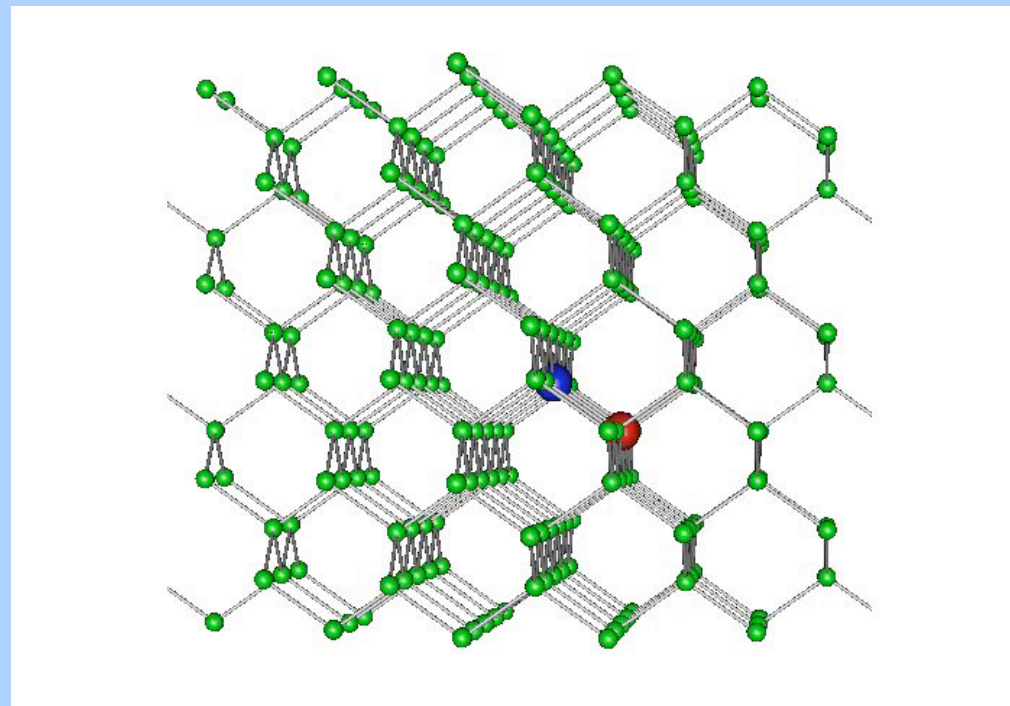
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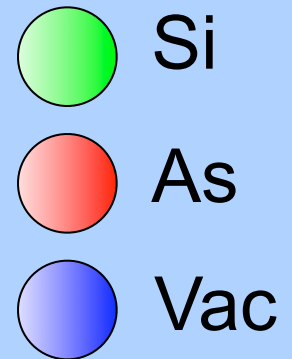
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# Problem with Kinetic Monte Carlo

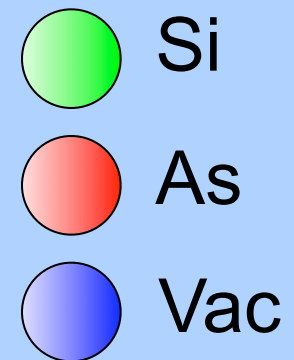
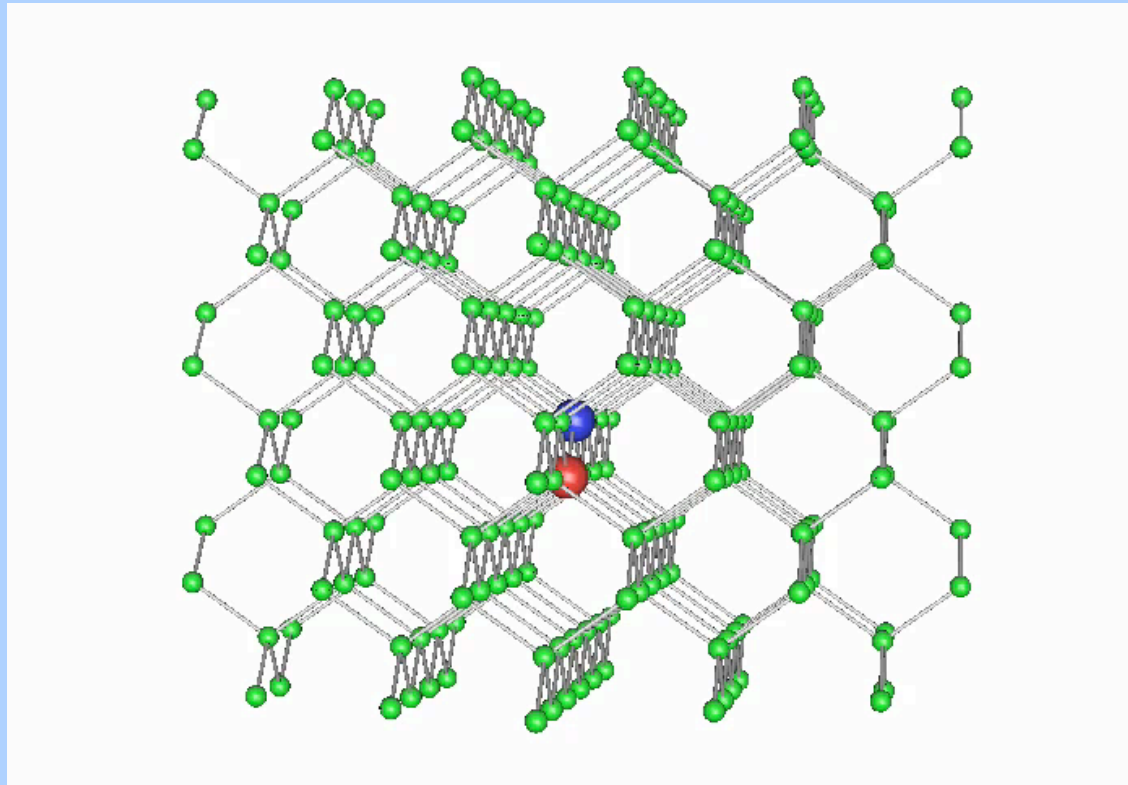
- Standard rejection free schemes are slow due to low barriers between various bound states.



- This problem is markedly worse for dopant clusters.

# Problem with Kinetic Monte Carlo

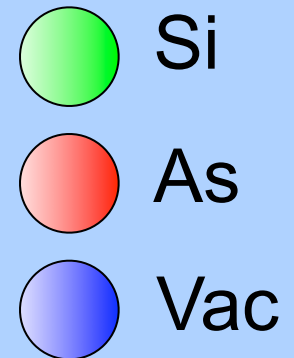
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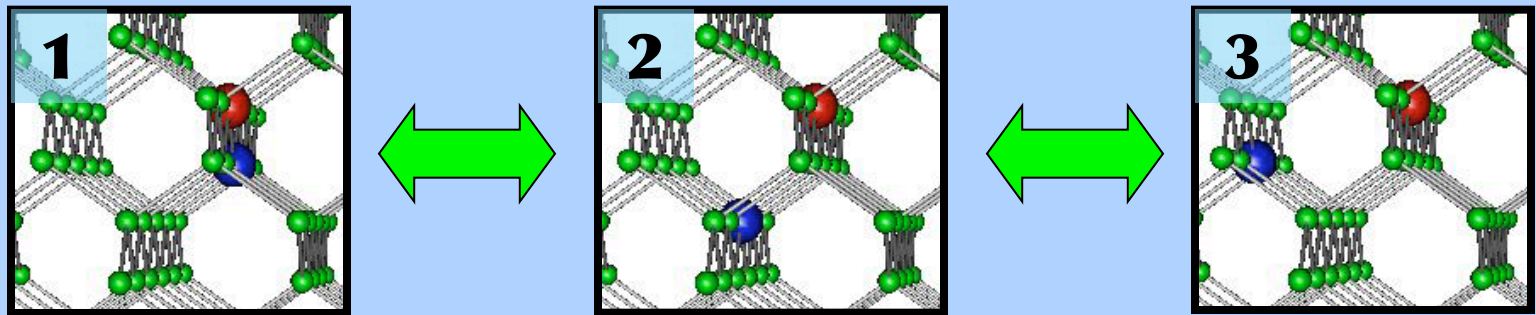
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# Accelerating Kinetic Monte Carlo

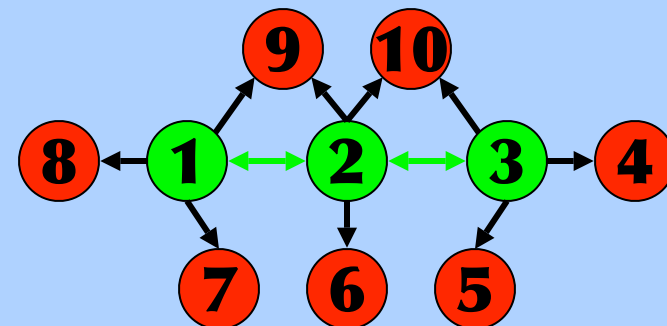
- As new configurations are explored store up to a maximum number of them in a graph of states we will call memorized states



- Rather than calculate the time to transition from the current state to an adjacent state, calculate the time to exit the entire graph of memorized states via any of the transitions out of this connected graph of states.

M. A. Novotny, *Phys. Rev. Lett.* 74 (1995) 1; Erratum, *Phys. Rev. Lett.* 75 (1995) 1424. (Ising Model)

C. S. Deo, D. J. Srolovitz, *Modelling Simul. Mater. Sci. Eng.* 10 (2002) 581. (Dislocation Kink Nucleation)





# First Passage Time in KMC

- Let the rate to transition from state p to state q be denoted  $r_{pq}$

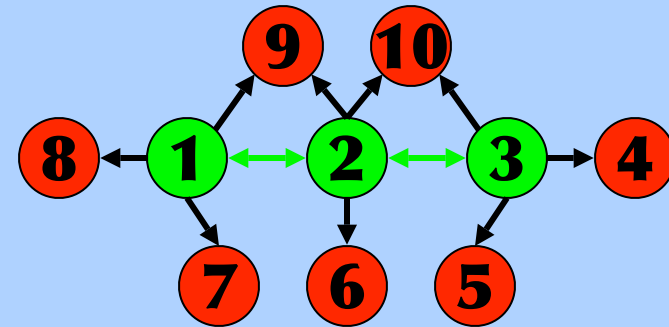
- Then we can define a matrix  $M_{ba} = \frac{r_{ab}}{\sum_n r_{bn}}$

- The time spent in each state prior to exiting the connected states is then

$$T = T^0 + T^1 + T^2 + \dots = T^0 + \mathbf{M}T^0 + \mathbf{M}^2T^0 + \dots$$

$$T = \left[ \sum_{n=0}^{\infty} \mathbf{M}^n \right] T^0 = [\mathbf{I} - \mathbf{M}]^{-1} T^0$$

$$T_s^0 = \frac{\delta_{si}}{\sum_k r_{sk}}$$

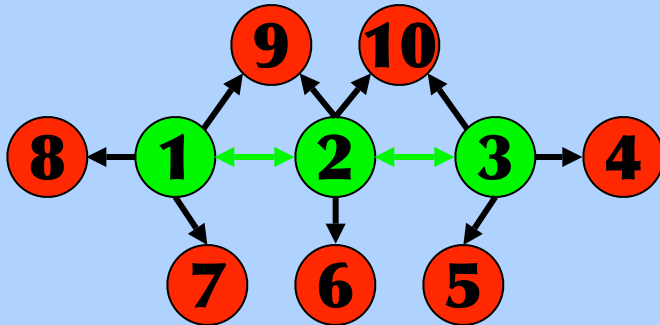


- T is a vector containing the average time spent in each state prior to exiting the memorized states.
- $T^0$  is the average time spent in each of the memorized states from time zero until the first jump.  $i$  = initial state
- This allows us to compute the net rate out via a transition from memorized state s to outside state j

$$R_{sj} = \frac{T_s r_{sj}}{\sum_n T_n}$$

# First Passage Time in KMC

- **Problem: The first passage time distribution is no longer a Poisson distribution.**



Master eq: 
$$\frac{\partial}{\partial t} P(n, t | n_0, t_0) = \sum_v (R(v \rightarrow n) P(v, t | n_0, t_0) - R(n \rightarrow v) P(n, t | n_0, t_0))$$

Solve diff. eq: 
$$\frac{\partial}{\partial t} \bar{P}(t) = -\bar{M} * \bar{P}(t)$$

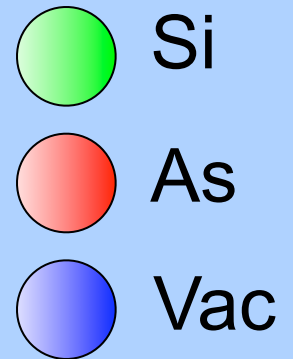
Molar, C., Van Loan, C., "Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later\*", SIAM REVIEW Vol. 45, No. 1, (2003).

$\lambda, V$  are eigenvalues/vectors: 
$$\bar{P}_{n_{final}}(t) = \sum_{j=1}^N \bar{V}_{n_{final}, j} * \bar{V}_{j, n_{init}}^{-1} * e^{-\lambda_j t}$$

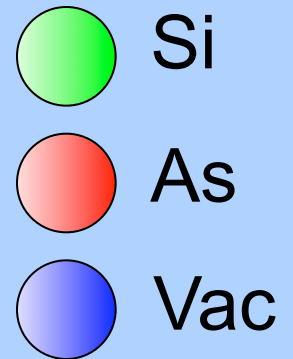
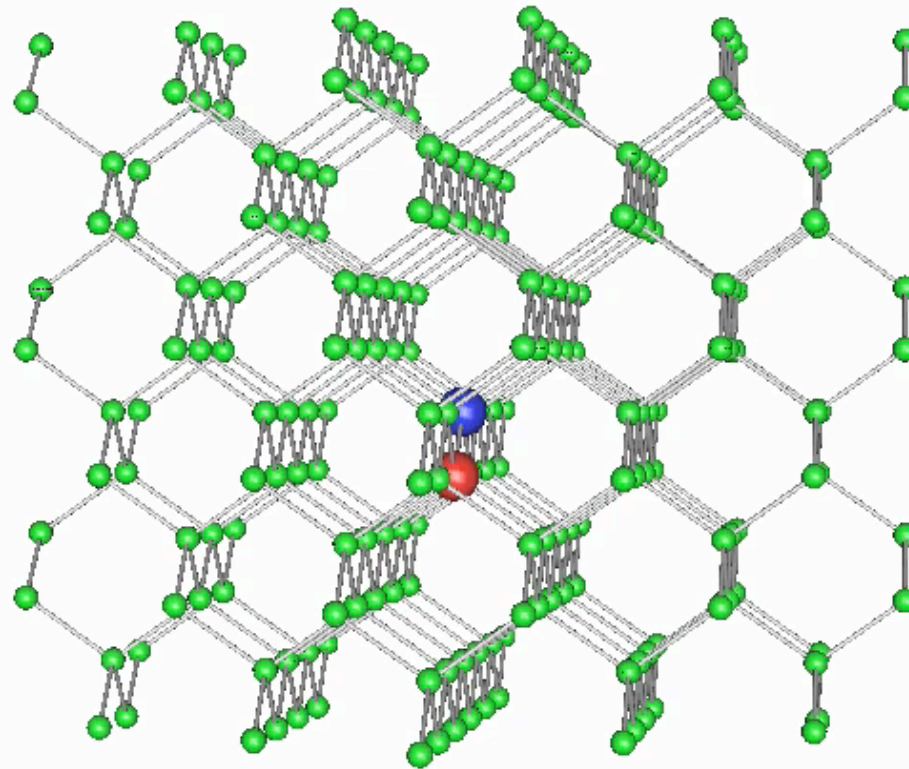
# Enumerating Saved States in KMC

- **We consider two methods to enumerate which states to save in a basin.**
  - **Jump First:** Successively add states as they are visited up to a predetermined number.
  - **Look First:** Define a basin by an analysis of the energy barriers between states.
- **We also implemented methods to save information regarding clusters of states, and to combine basins into larger basins if transitions between basins recur.**

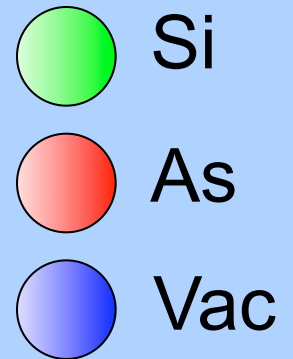
# Example: Single Dopant



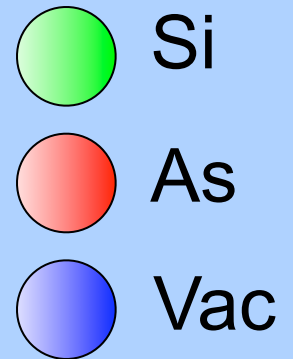
# Example: Single Dopant



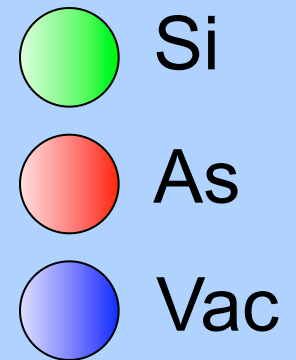
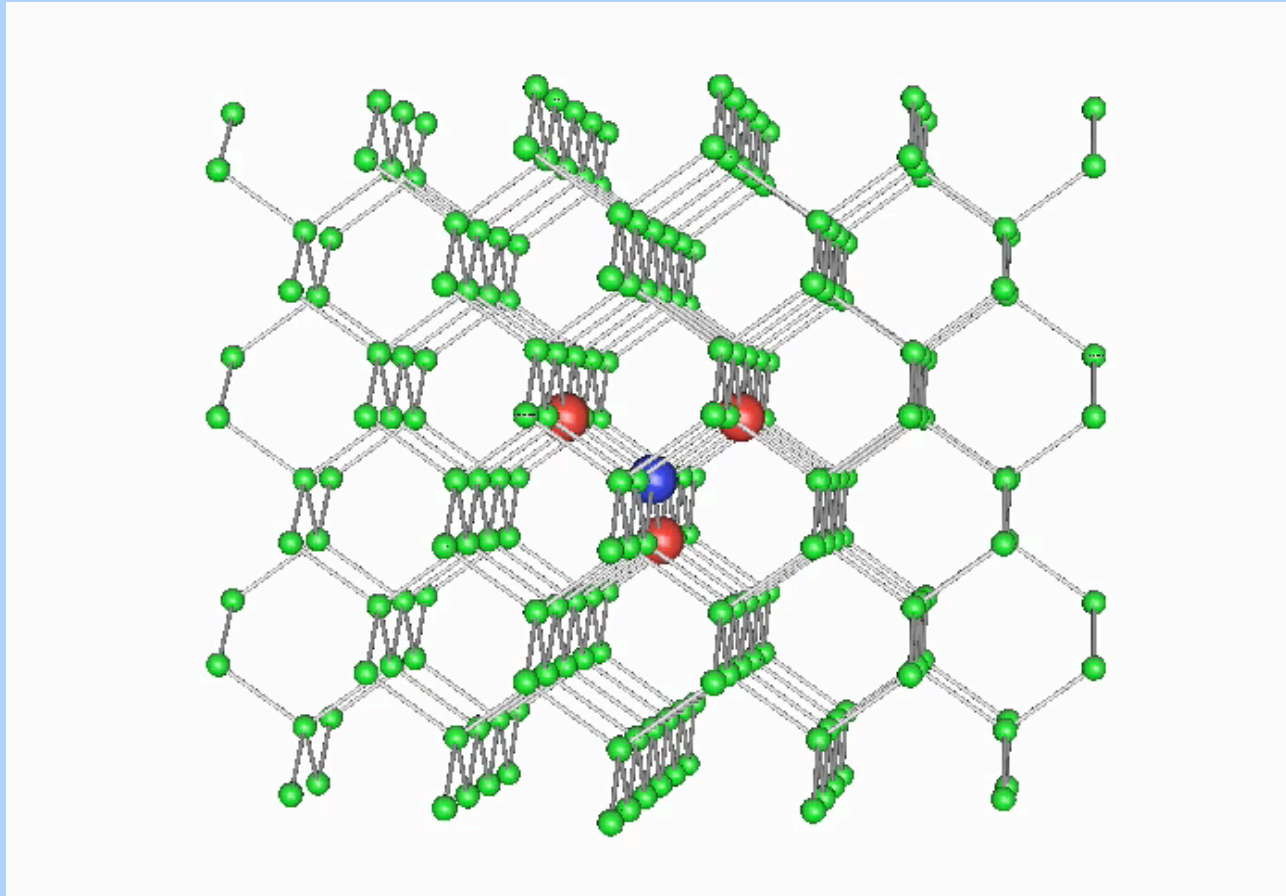
# Example: Single Dopant



# Example: 3 Dopant Cluster



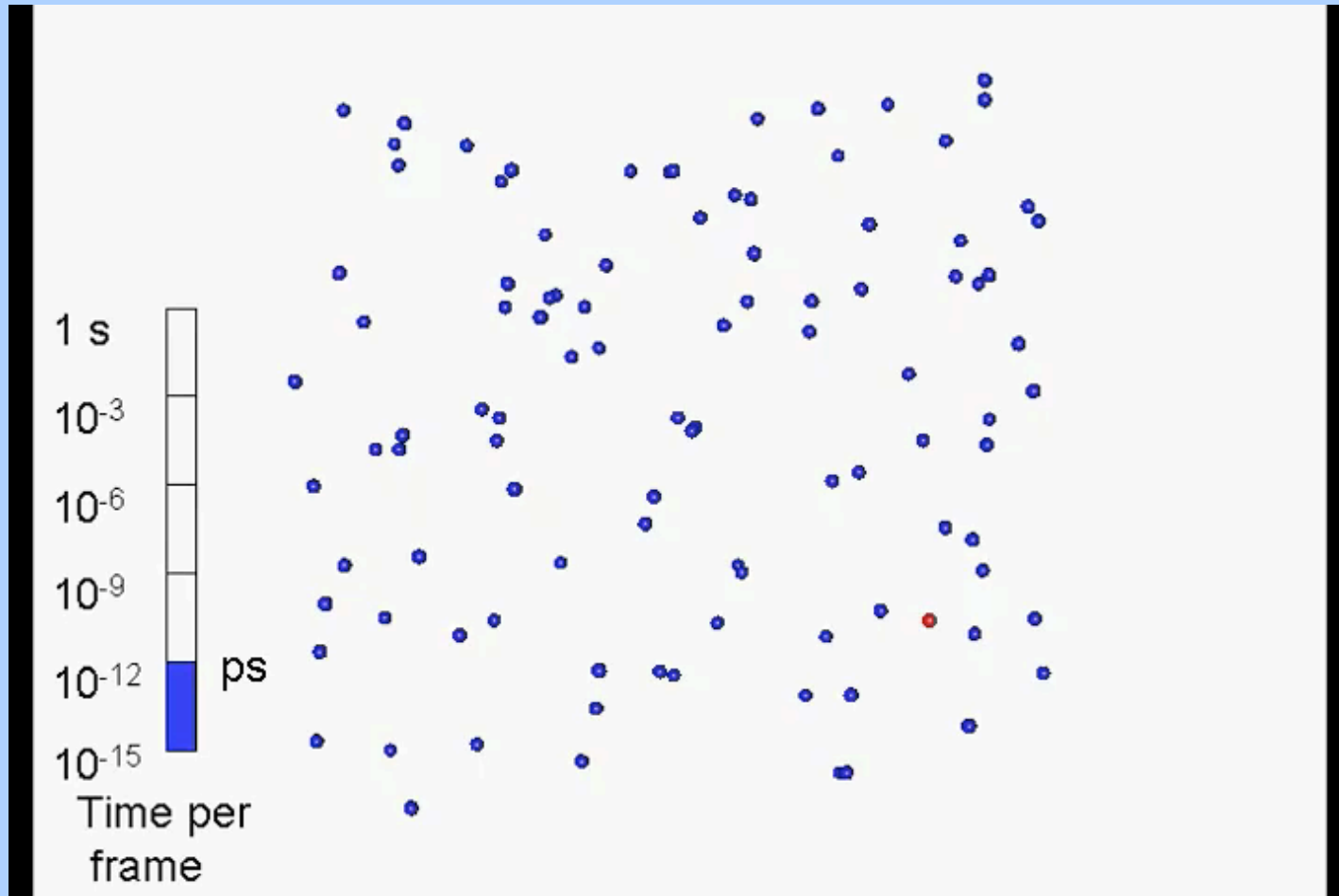
# Example: 3 Dopant Cluster





# Traversing Time Scales

512,000 lattice positions, (22nm on a side), 1Vac, 100As  
 $c_V=10^{17}\text{cm}^{-3}$   $c_{As}=10^{19}\text{cm}^{-3}$



# Promise and Limitations of Accelerated KMC

- Novel algorithm for speeding up Kinetic Monte Carlo without arbitrary approximations.
- Overcomes the time scale limitations of other simulation methodologies
- **Minutes of simulated time!**
- Useful for understanding diffusion dynamics, ie percolation diffusion.
- **Future Directions**
  - Apply to evolution of nanostructures such as quantum dots, thermoelectrics and intercalated compounds found in batteries

- Limited to systems where we can enumerate the transitions a priori
- Not suitable for disordered materials or systems in which transitions are highly complex or where their activation energies are difficult to compute

# Accelerating Molecular Dynamics

- **Arthur Voter at LANL proposed 3 methods for simulating activated processes using creative approaches to MD simulation to access longer time scales**
  - Parallel Replica Dynamics
  - Temperature Accelerated Dynamics
  - Hyperdynamics
- **I will discuss all three, but will spend the most time on hyperdynamics, which is a subject of my current research.**

# Parallel Replica Dynamics

- Parallel Replica Dynamics utilizes only the fact that we expect our activated processes to be Poisson processes.
- The system starts in some state.
- Replicate that structure across  $P$  processors, but randomize the initial momenta of particles from a Boltzmann distribution appropriate for the temperature.
- Simulate for enough time to decorrelate the systems,  $t_d$ .
- Periodically check for transitions and determine how much time elapses before the first transition takes place,  $t_t$ .
- Advance clock by  $P \times t_t$ .
- Assuming checking for transitions, replicating and randomizing are of negligible speedup  $\sim P \left( 1 - \frac{P}{1 + \frac{t_t}{t_d}} \right)$

# Temperature Accelerated Dynamics

- Assume harmonic transition state theory.
- Also assume all transitions have the same (or a known) attempt frequency.
- Run system at high temperature; things happen faster!
- But don't accept the first transition. When you detect the transition reflect the system back into the well and wait for a second transition.
- Measure the each energy barrier by examining the lowest energy path connecting the minimum to the final state.
- From this we can calculate when they would have happened at the lower target temperature.

# Temperature Accelerated Dynamics

- Since this is a Poisson process

$$f_i(t)dt = R_i \exp(-R_i t) dt$$

- From this we can infer the time the event would have occurred at low T from the time it occurred at high T

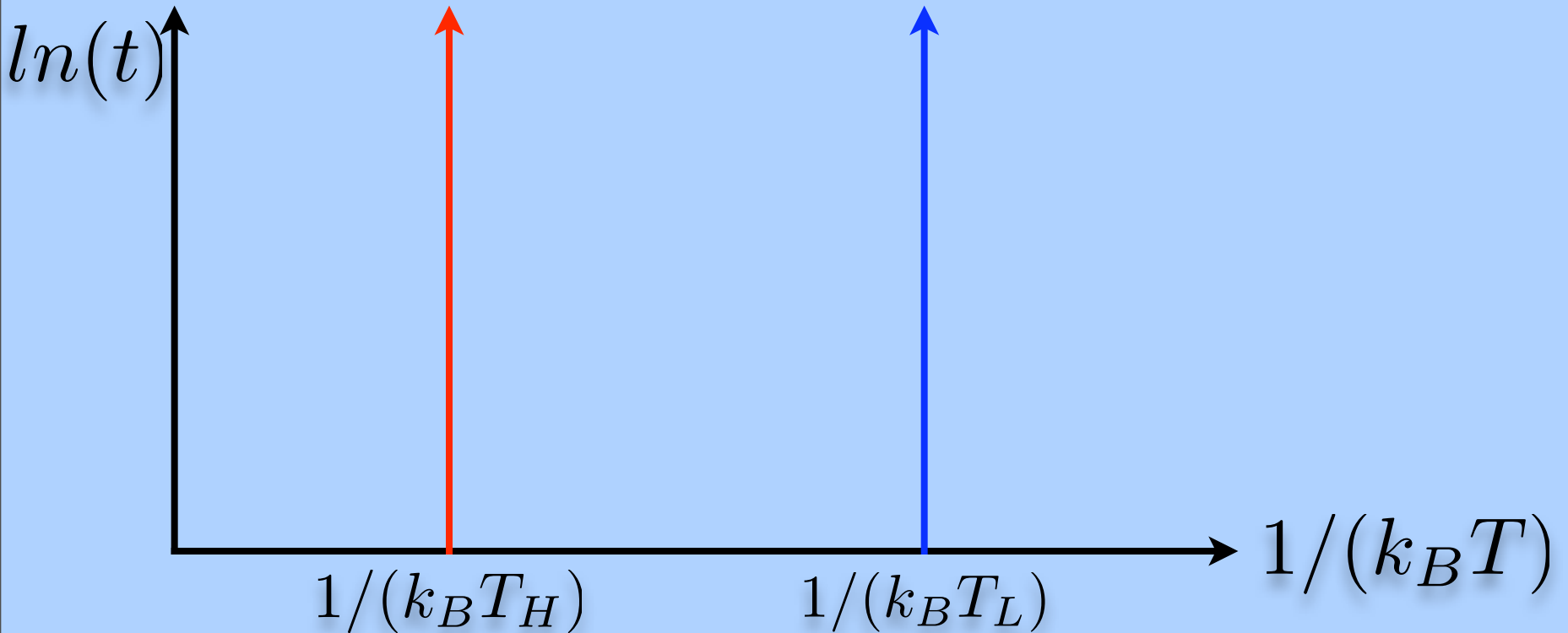
$$t_L R_L = t_H R_H \qquad t_L = t_H \frac{\exp\left(-\frac{E_i}{k_B T_H}\right)}{\exp\left(-\frac{E_i}{k_B T_L}\right)}$$

$$t_L = t_H \exp\left[E_i \left(\frac{1}{k_B T_L} - \frac{1}{k_B T_H}\right)\right]$$

$$\ln(t_L) = \ln(t_H) + E_i \left(\frac{1}{k_B T_L} - \frac{1}{k_B T_H}\right)$$

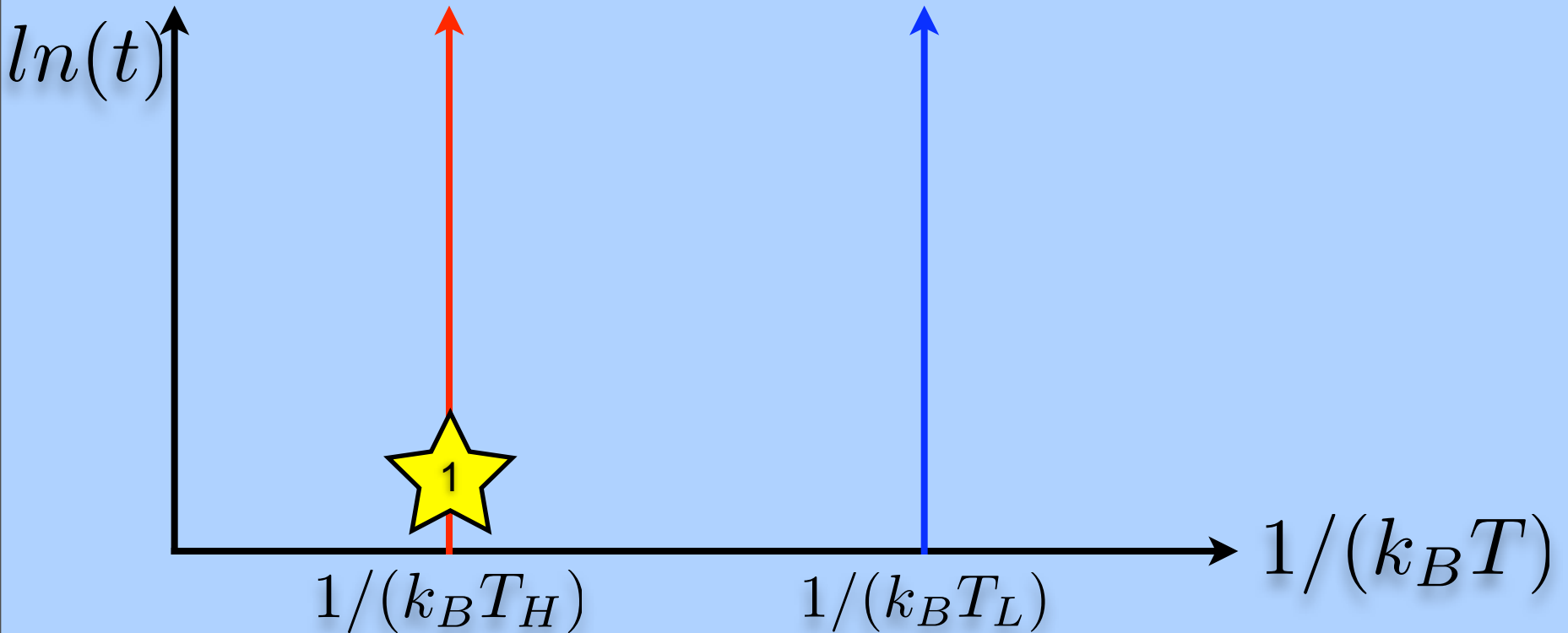
# Temperature Accelerated Dynamics

$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



# Temperature Accelerated Dynamics

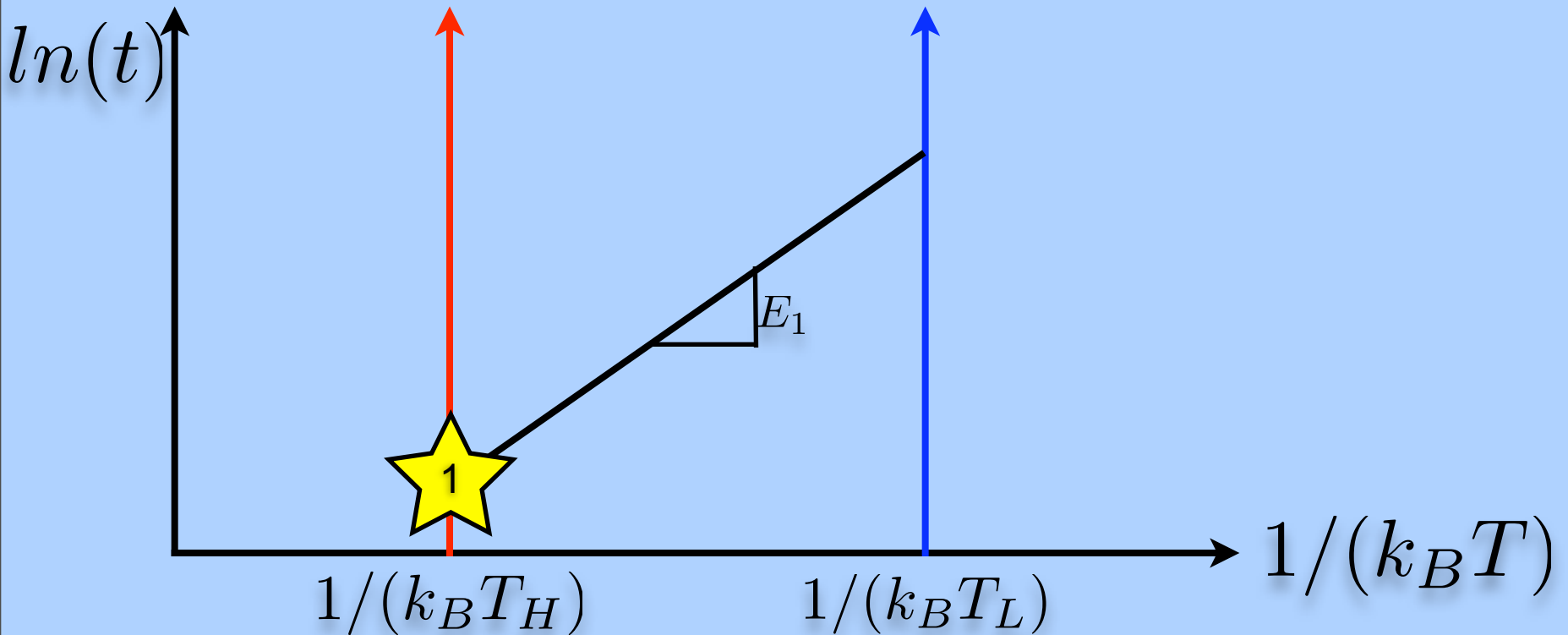
$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$





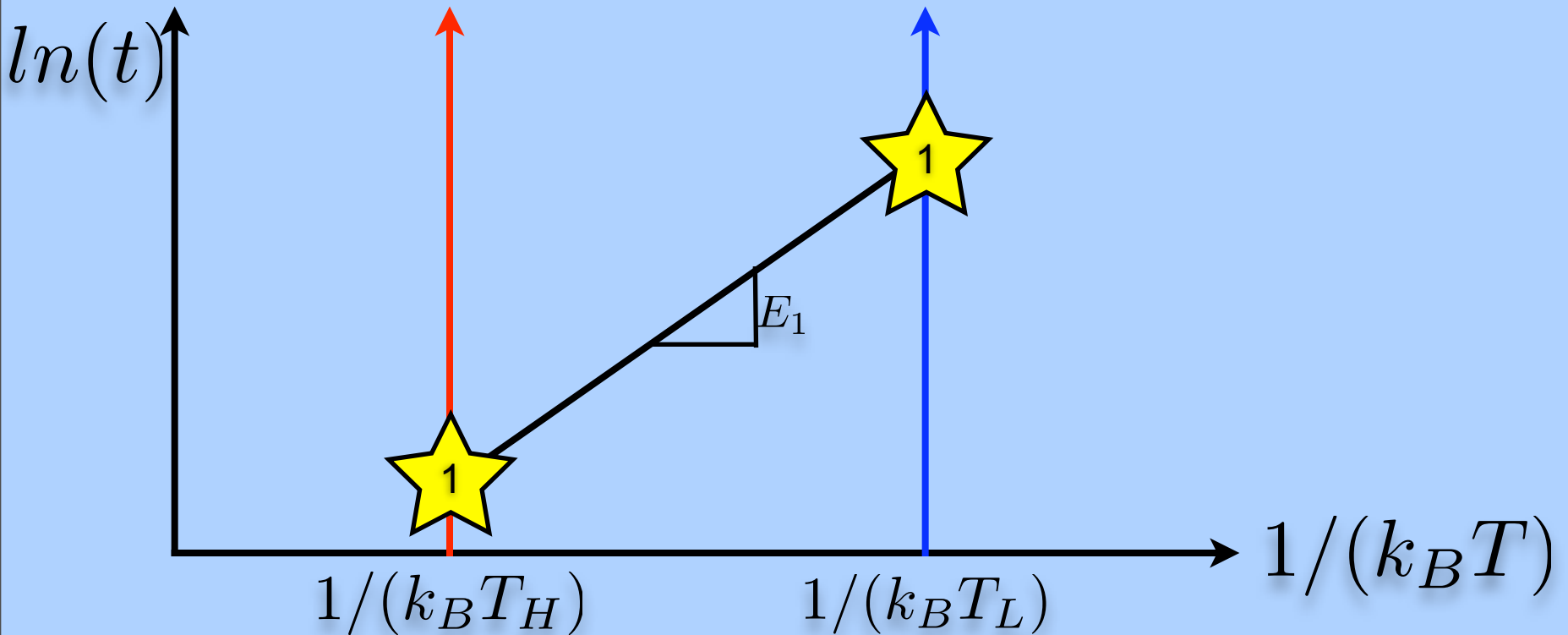
# Temperature Accelerated Dynamics

$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



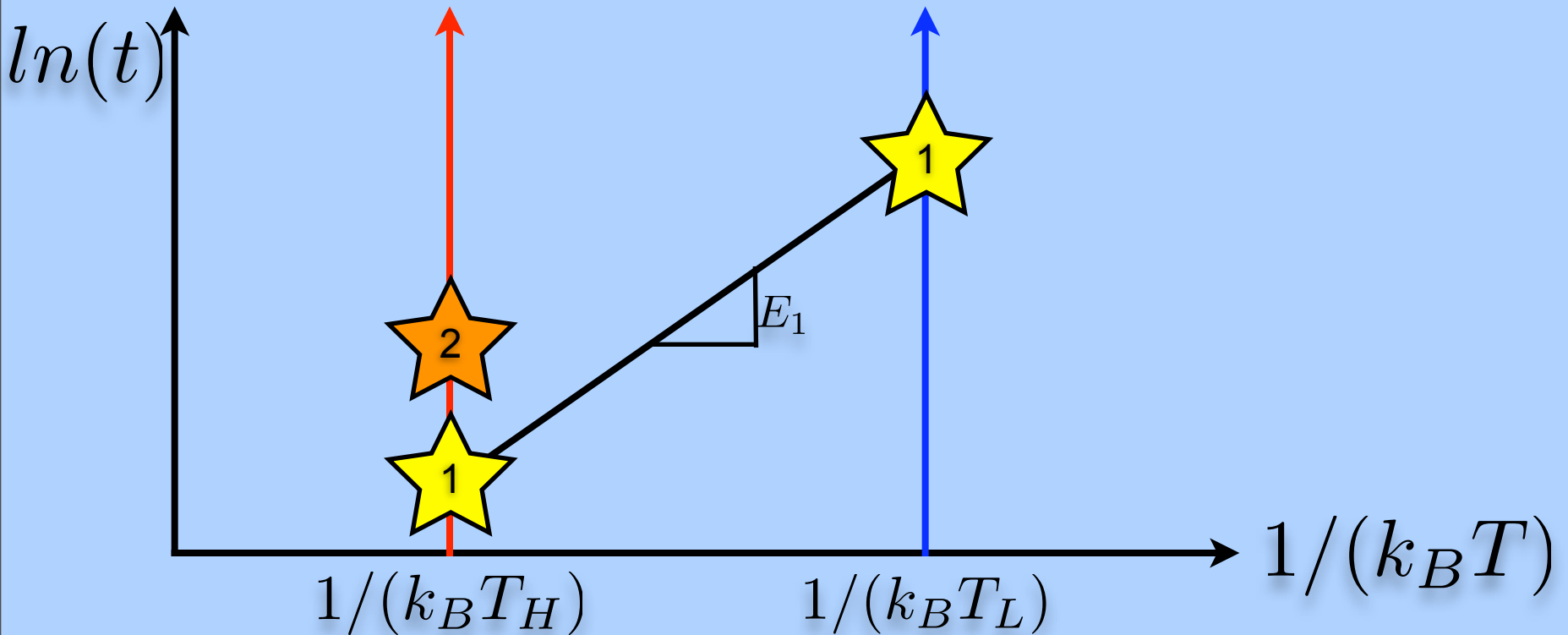
# Temperature Accelerated Dynamics

$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



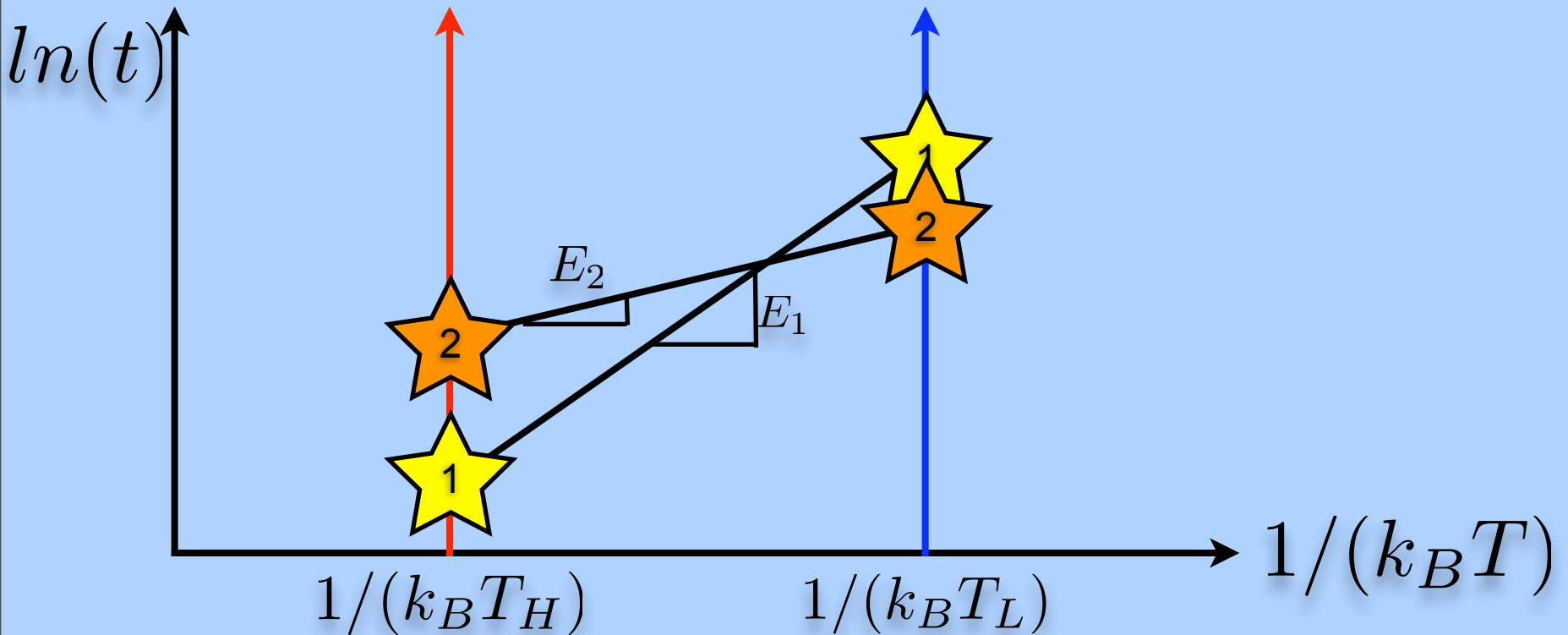
# Temperature Accelerated Dynamics

$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



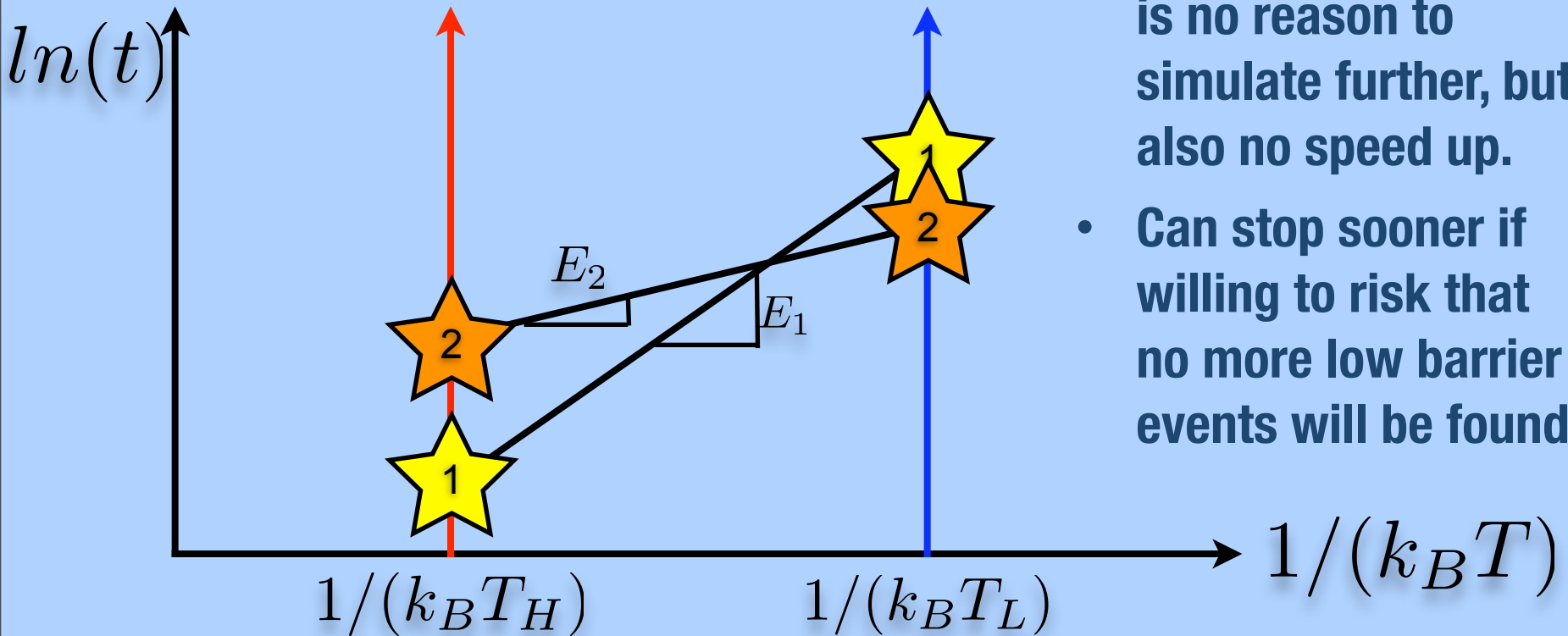
# Temperature Accelerated Dynamics

$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



# Temperature Accelerated Dynamics

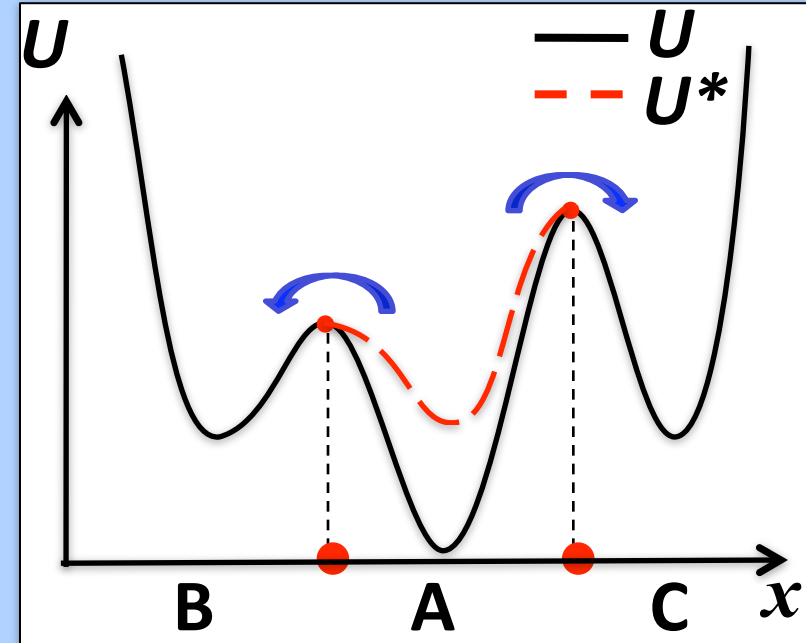
$$\ln(t_L) = \ln(t_H) + E_i \left( \frac{1}{k_B T_L} - \frac{1}{k_B T_H} \right)$$



- If  $t$  is less greater than the first known event at low  $T$  there is no reason to simulate further, but also no speed up.
- Can stop sooner if willing to risk that no more low barrier events will be found.

# Hyperdynamics (HD)

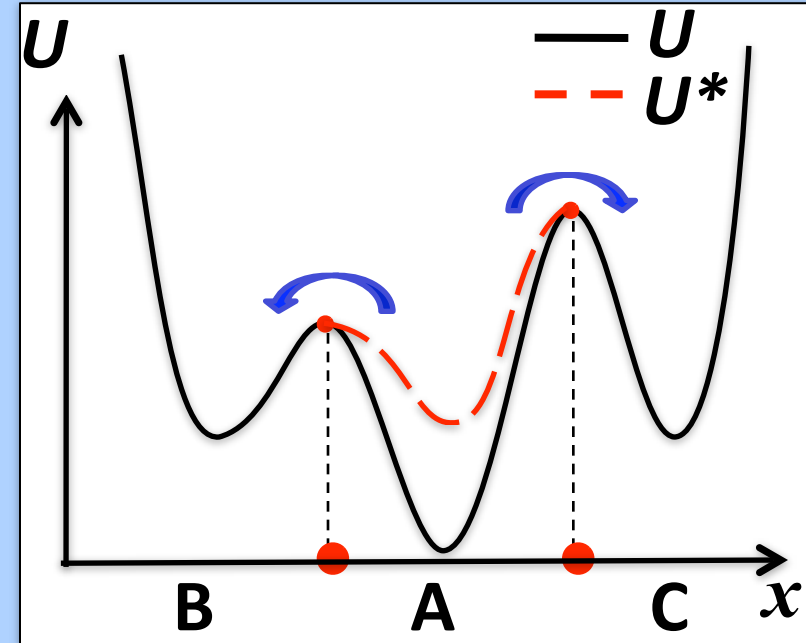
- HD starts from a TST hypothesis
- Within TST something interesting happens if you can create a new potential related to the original potential in the following ways:
  - The new potential is higher in the vicinity of the current minimum
  - The new potential does not create any new minima that did not exist before
  - The new potential goes to zero at all dividing surfaces that separate the current minimum from neighboring minima.



(Voter, J. Chem. Phys., 1997)

# Transition State Theory

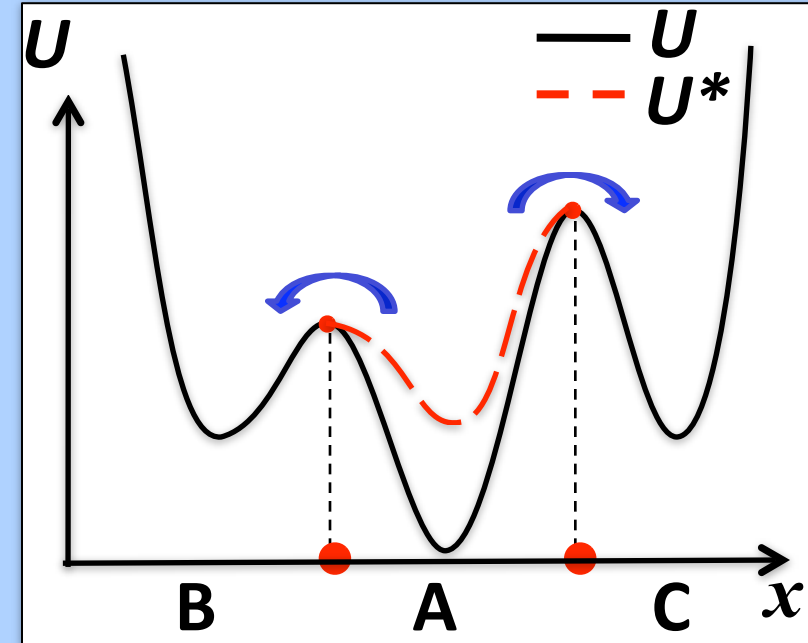
- Note that in our expression for the TST rate given below only the denominator depends on the potential in the well
- The numerator is preserved by construction of the boost potential



$$R_{A \rightarrow B} \approx \frac{\int dr^{3N-1} \int_{-\infty}^{\infty} dv^{3N} (\vec{v} \cdot \hat{n}) \Theta(\vec{v} \cdot \hat{n}) \exp\left(-\frac{\frac{1}{2}mv^2 + U(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \int_{-\infty}^{\infty} dv^{3N} \exp\left(-\frac{\frac{1}{2}mv^2 + U(\vec{r})}{k_B T}\right)}$$

# Calculating the Boost

- Assuming all these conditions hold, it is evident that the rates of transition out of the current state will be faster.
- How much faster?



(Voter, J. Chem. Phys., 1997)

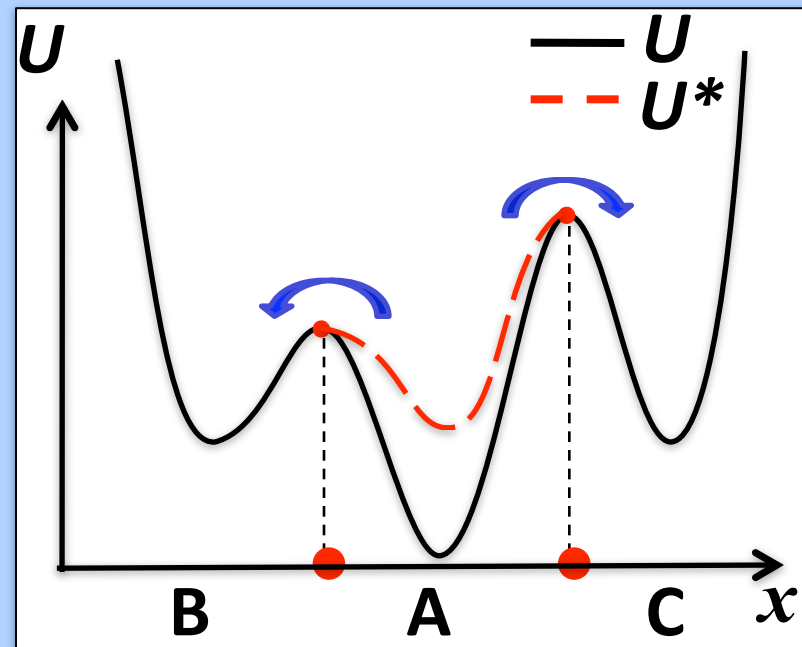
$$\langle t_{esc} \rangle = \beta \times \langle t_{esc} \rangle^*$$

$$\beta = \frac{R_{A^* \rightarrow B}}{R_{A \rightarrow B}} = \frac{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)} = \frac{\int_{\Omega_A} dr^{3N} \exp\left(\frac{\Delta U(\vec{r})}{k_B T}\right) \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)} = \langle e^{\Delta U / k_B T} \rangle^*$$



# Physics is Preserved

- Note that all exit rates are boosted by the same factor
- This preserves the original physics since the relative probabilities of all possible events are the same
- This “**boost factor**” allows us to accomplish the same simulation in much less time.



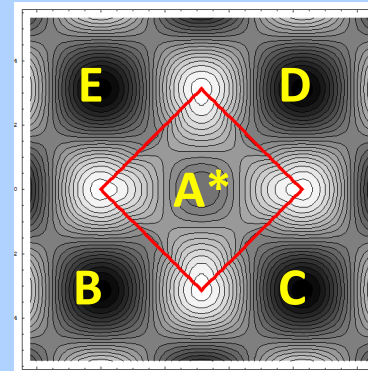
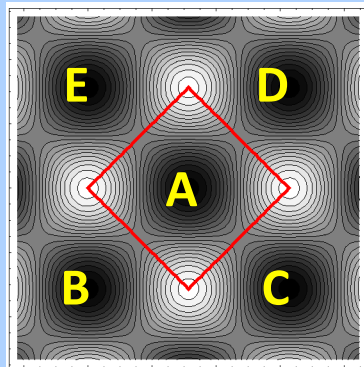
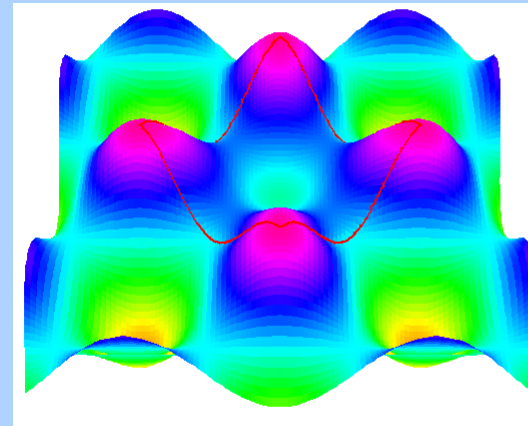
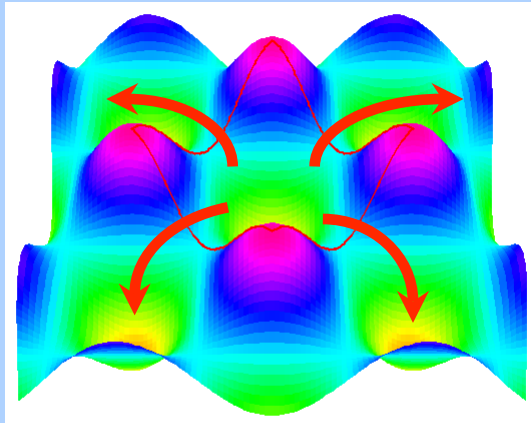
(Voter, J. Chem. Phys., 1997)

$$\langle t_{esc} \rangle = \beta \times \langle t_{esc} \rangle^*$$

$$\beta = \frac{R_{A^* \rightarrow B}}{R_{A \rightarrow B}} = \frac{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)} = \frac{\int_{\Omega_A} dr^{3N} \exp\left(\frac{\Delta U(\vec{r})}{k_B T}\right) \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)}{\int_{\Omega_A} dr^{3N} \exp\left(-\frac{U^*(\vec{r})}{k_B T}\right)} = \langle e^{\Delta U / k_B T} \rangle^*$$

# Defining a Boost Potential

- Defining a proper boost potential is non-trivial

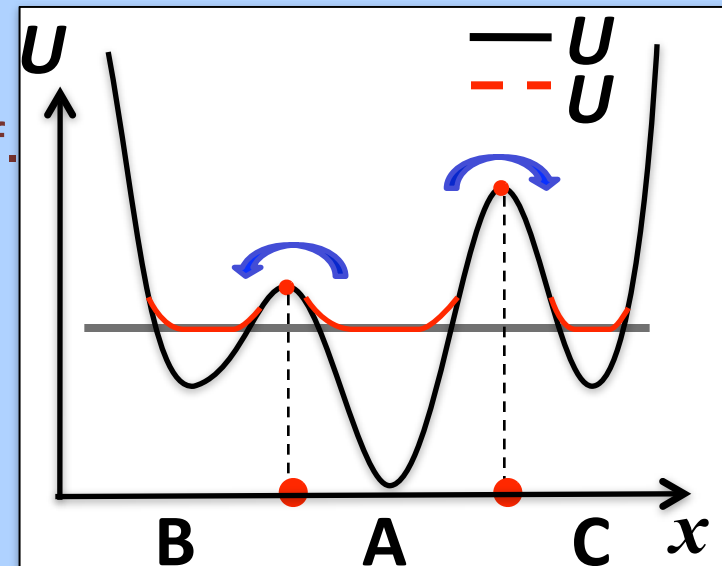


- **Voter's original bias potential**

- The lowest eigenvalue  $\epsilon$  of the Hessian  $\mathbf{A}_{ij} = \frac{\partial^2 U}{\partial \vec{r}_i \partial \vec{r}_j}$
- $\epsilon > 0$  : biased region ( $\Delta V > 0$ )
- $\epsilon < 0$  : unbiased region ( $\Delta V = 0$ )
- Eigenvalues are expensive to calculate!!!
- Forces require 3rd derivative of energy.

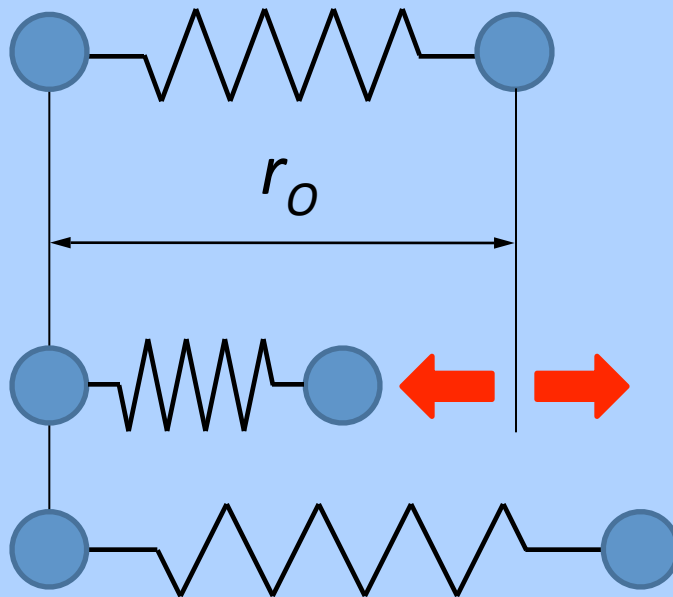
- **Steiner, Genilloud and Wilkins**

- Turn off the potential below some cutoff.
- Simple, but need to know the minimum energy of barrier



# Bond-Boost Method

(Miron and Fichthorn, J. Chem. Phys., 2003)



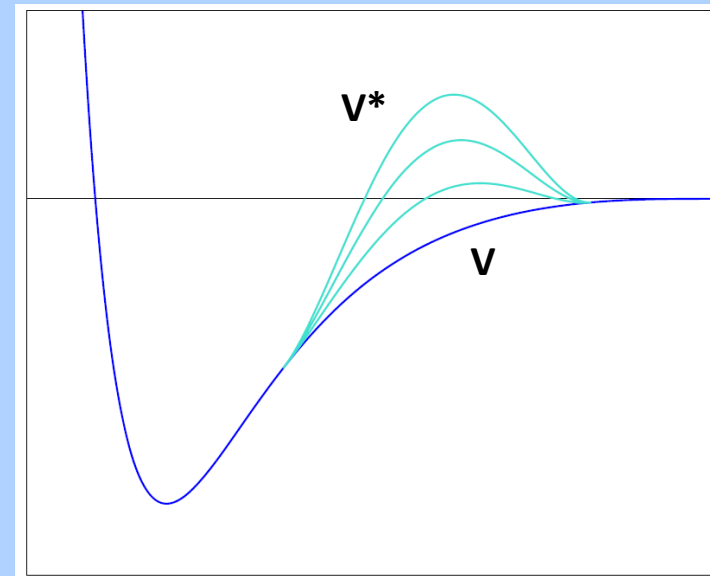
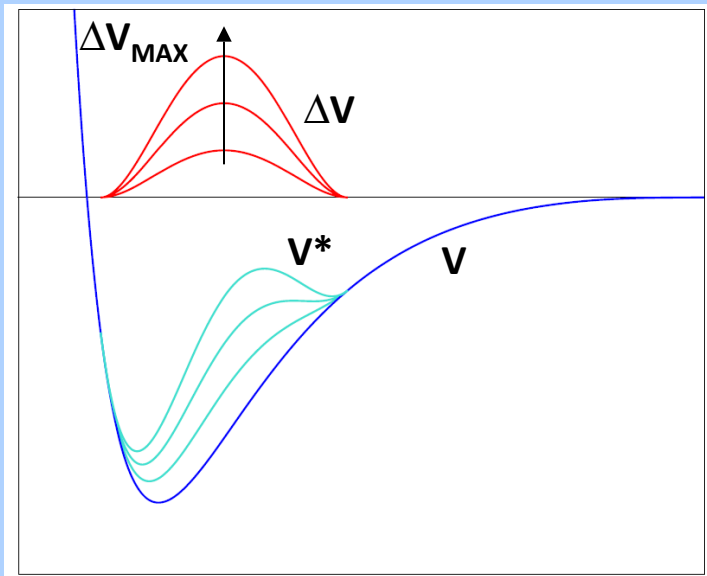
$$\varepsilon = \frac{r - r_0}{r_0}$$

$$\Delta V = A(\varepsilon_{\max}) \sum_i \delta V(r_i)$$
$$\delta V(r_i) = \begin{cases} C \left( 1 - \left( \frac{\varepsilon_i}{q} \right)^2 \right) & \text{if } |\varepsilon_i| < q \\ 0 & \text{if } |\varepsilon_i| \geq q \end{cases}$$

- When a bond stretches or compresses out of critical range from a reference length ( $|\varepsilon| > q$ ), the boost energy goes to zero.
- It works well in some cases, but has limitations.

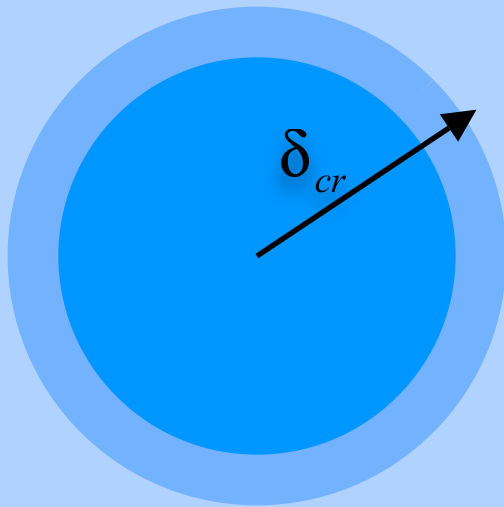
# Problems with Bond-Boost

- May create spurious minima
- May boost bond-breaking, but not bond-creation
- Currently developing more robust methods.



# Our Bias Potential

- Utilize the distance from the nearest local minimum in potential energy



$$\delta(\vec{r}) = |\vec{r} - \vec{r}_o| = \sqrt{\sum_{k=1}^{3N} (r_k - r_{o,k})^2}$$

$$\Delta V(\vec{r}) = \Delta V(\delta(\vec{r}))$$

$\delta < \delta_{cr}$  : biased region ( $\Delta V > 0$ )

$\delta > \delta_{cr}$  : unbiased region ( $\Delta V = 0$ )

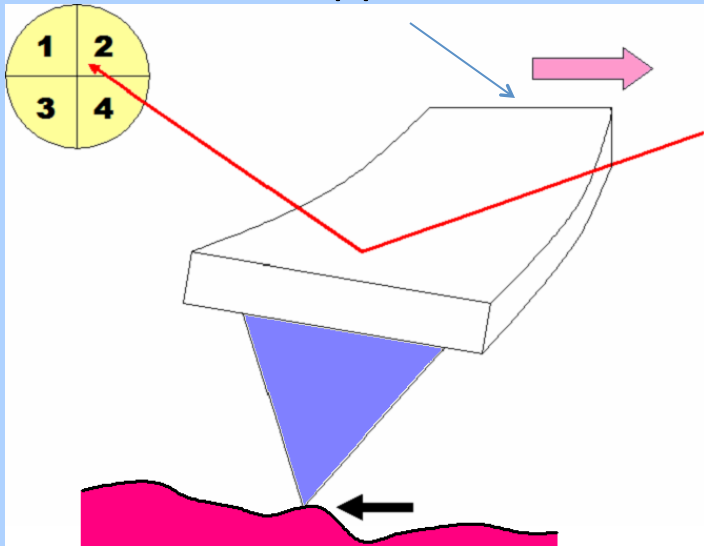
**➔ Only negligible computational overhead !!!**

# Studying Nano-friction

## AFM

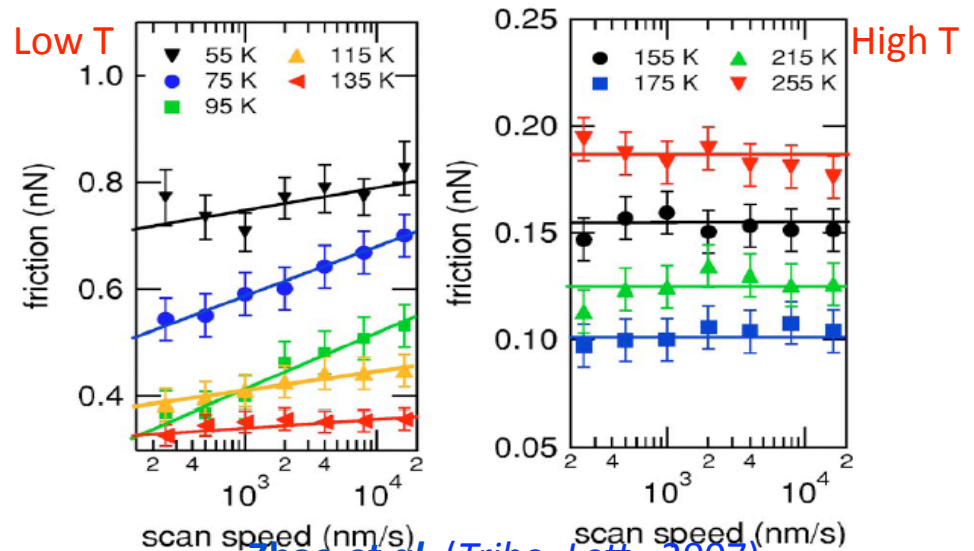
$$V_s = 10^2 \sim 10^4 \text{ nm/s}$$

supporter



Schirmeisen *et al.* (*Appl. Phys. Lett.*, 2006)

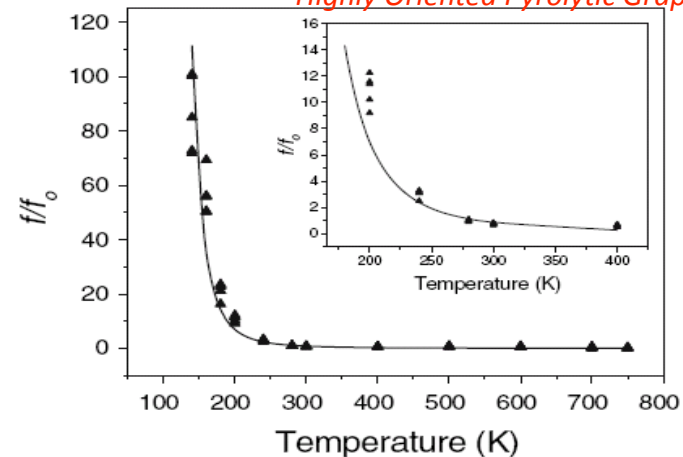
Silicon tip on a silicon surface with native oxides (UHV)



Zhao *et al.* (*Tribo. Lett.*, 2007)

$\text{Si}_3\text{N}_4$  tip on an HOPG surface (UHV)

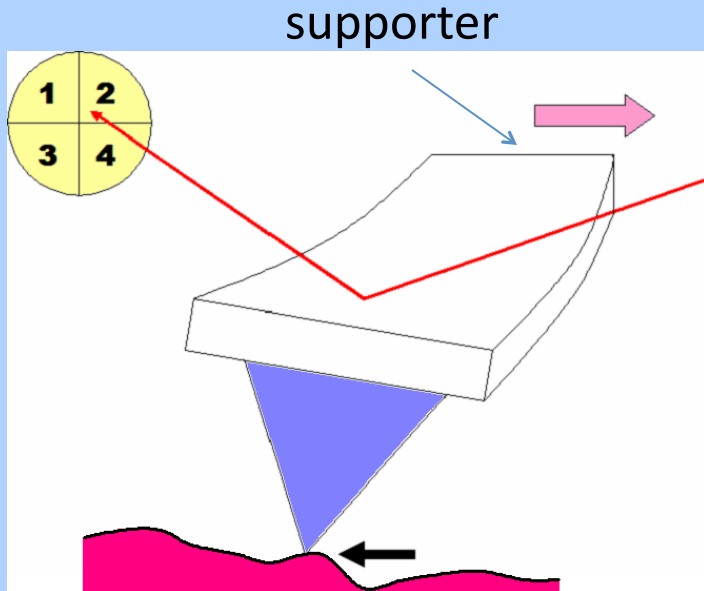
Highly Oriented Pyrolytic Graphite



# Simulating Nano-friction

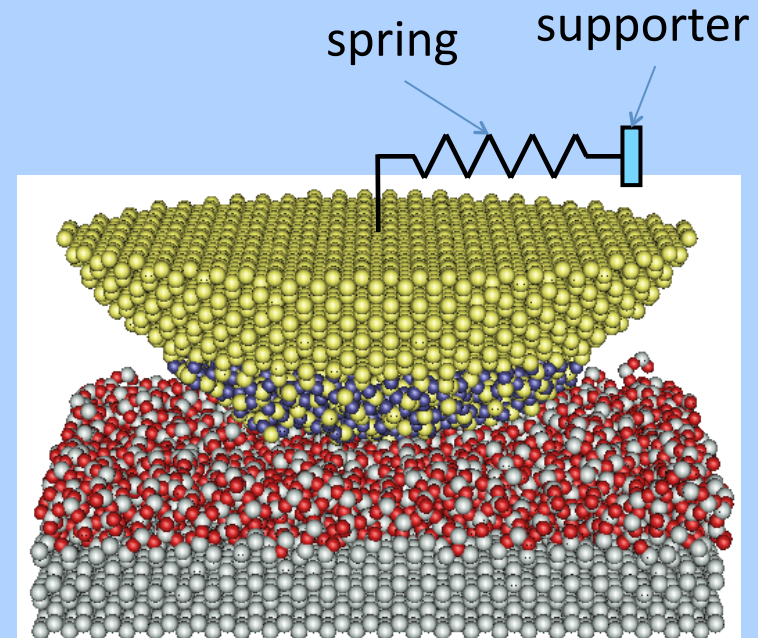
## AFM

$$V_s = 10^2 \sim 10^4 \text{ nm/s}$$



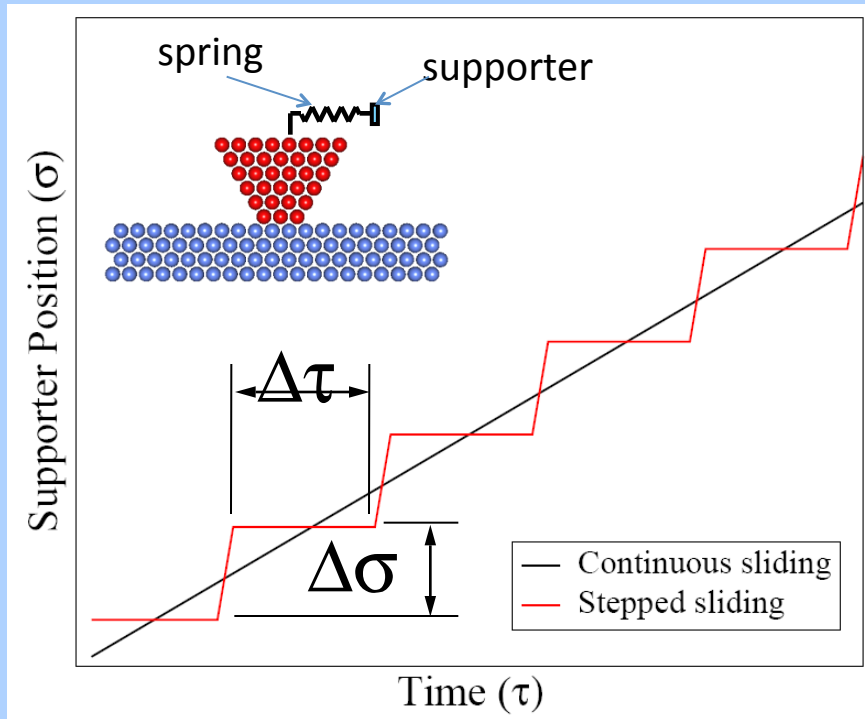
## MD

$$V_s = 10^7 \sim 10^{10} \text{ nm/s}$$



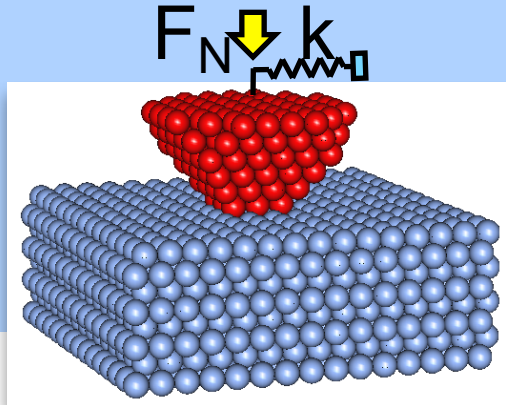


# Applying an Equilibrium Method to a Non-Equilibrium Problem

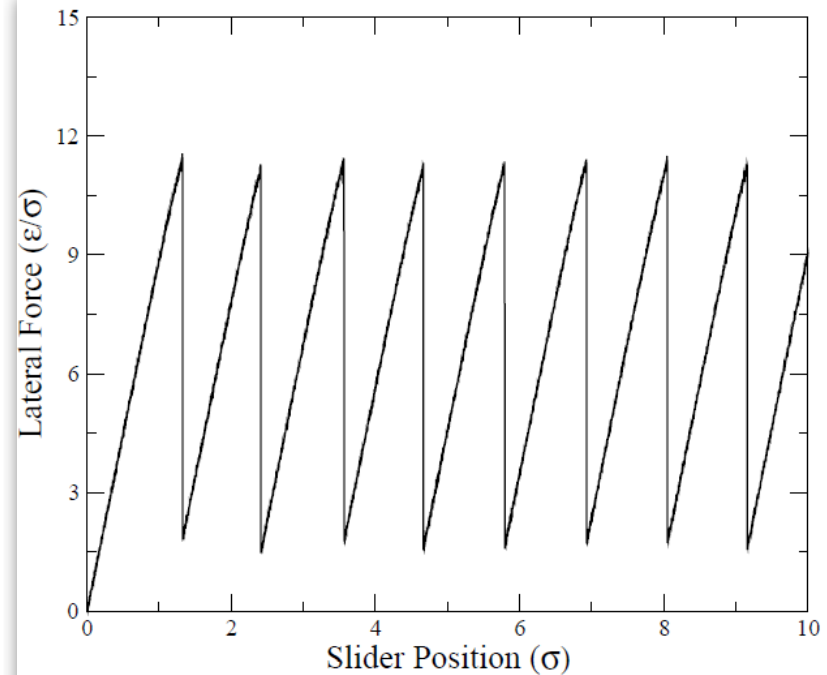
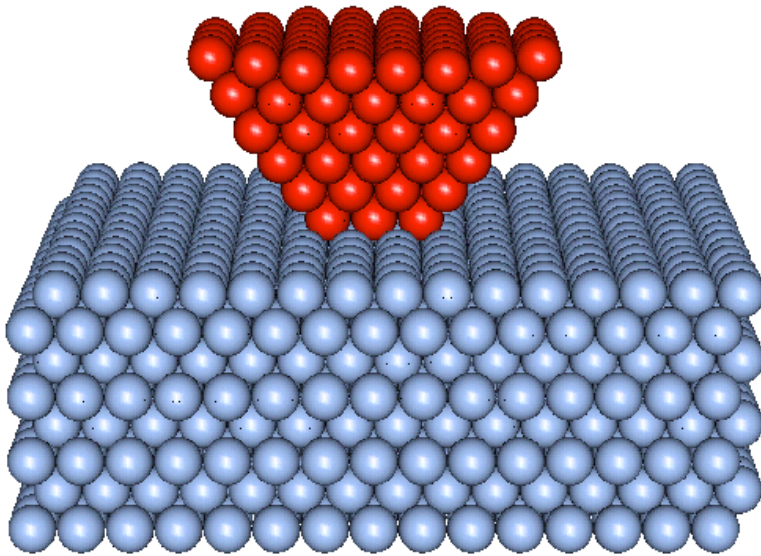


- We must hold the supporter position constant during boosting
- Periodically we update the slider position
- $v_s = \Delta\sigma/\Delta\tau$
- $\Delta\tau$  must be much greater than the attempt frequency
- $\Delta\tau$  must be much less than the rate of transitions.

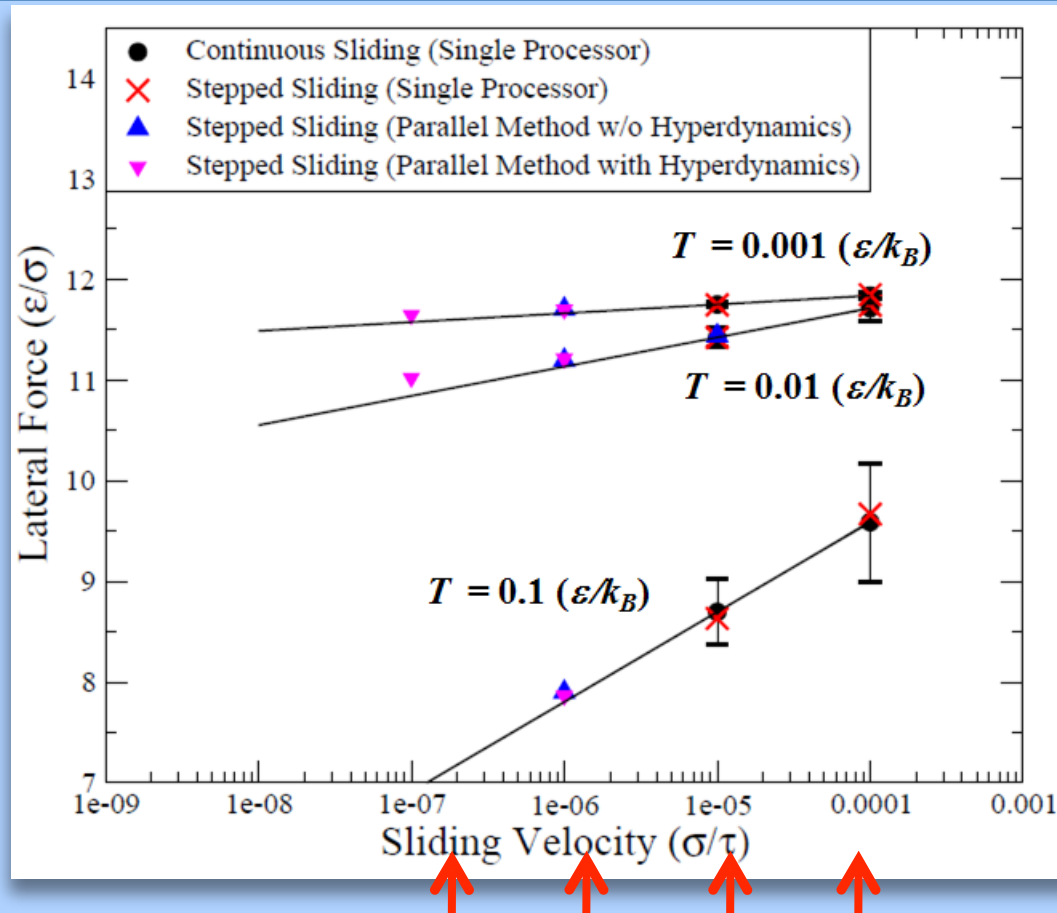
# Test System: 3D LJ Model



$$V(r) = 4\epsilon_{ab} \left[ \left( \frac{\sigma_{ab}}{r} \right)^{12} - \left( \frac{\sigma_{ab}}{r} \right)^6 \right]$$



# 3D LJ Model: Results



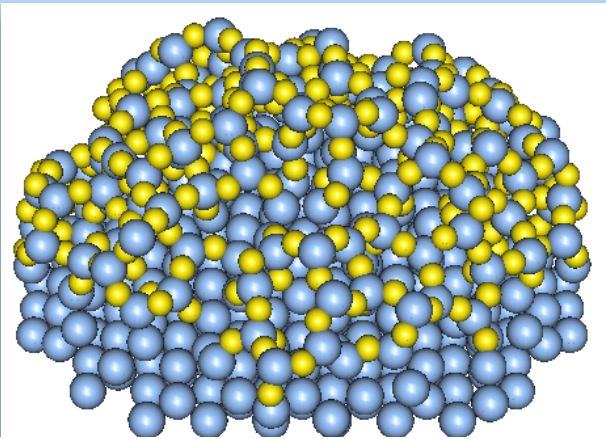
$$F \sim \ln(v_s)$$

Tomlinson  
Model  
(Gnecco, *PRL*,  
2000)

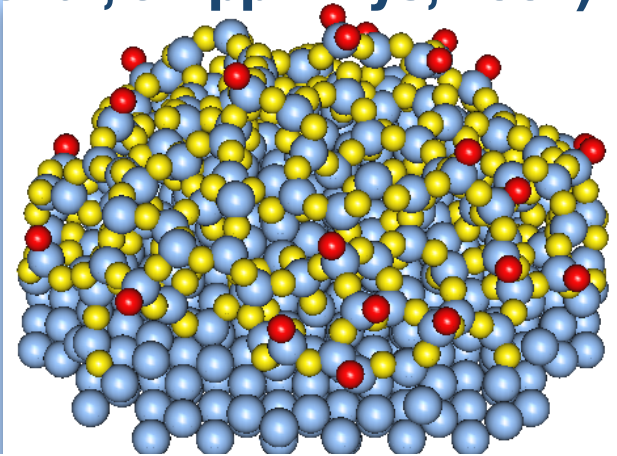
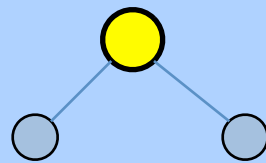
Conventional Method (hrs)	(30000)	(3000)	300	30
Parallel Method w/o HD (hrs)	(1500)	150	15	-
Parallel Method with HD (hrs)	190	130	-	-

# Friction of Silica Surfaces

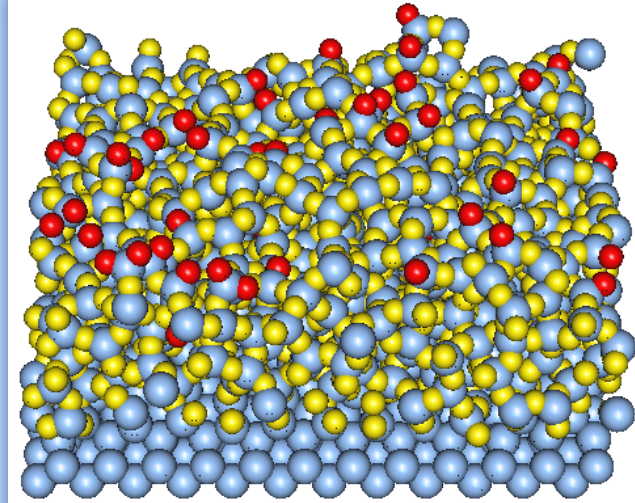
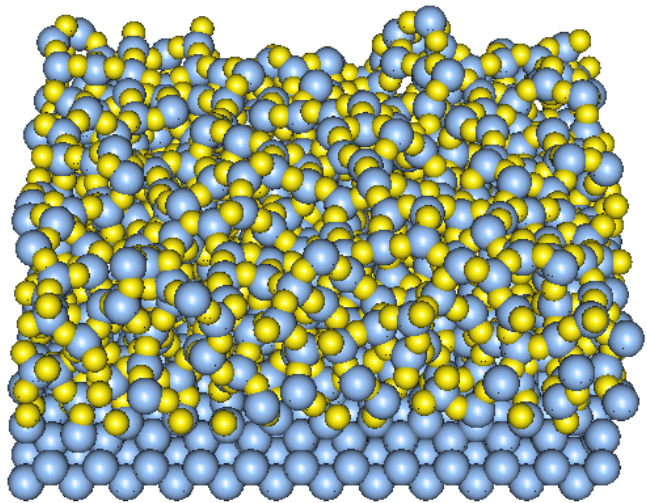
- Modified Stillinger-Weber potential (Watanabe, Jpn J Appl Phys, 1999)
- Dalla Torre's oxidation procedure (Dalla Torre et al, J Appl Phys, 2002)



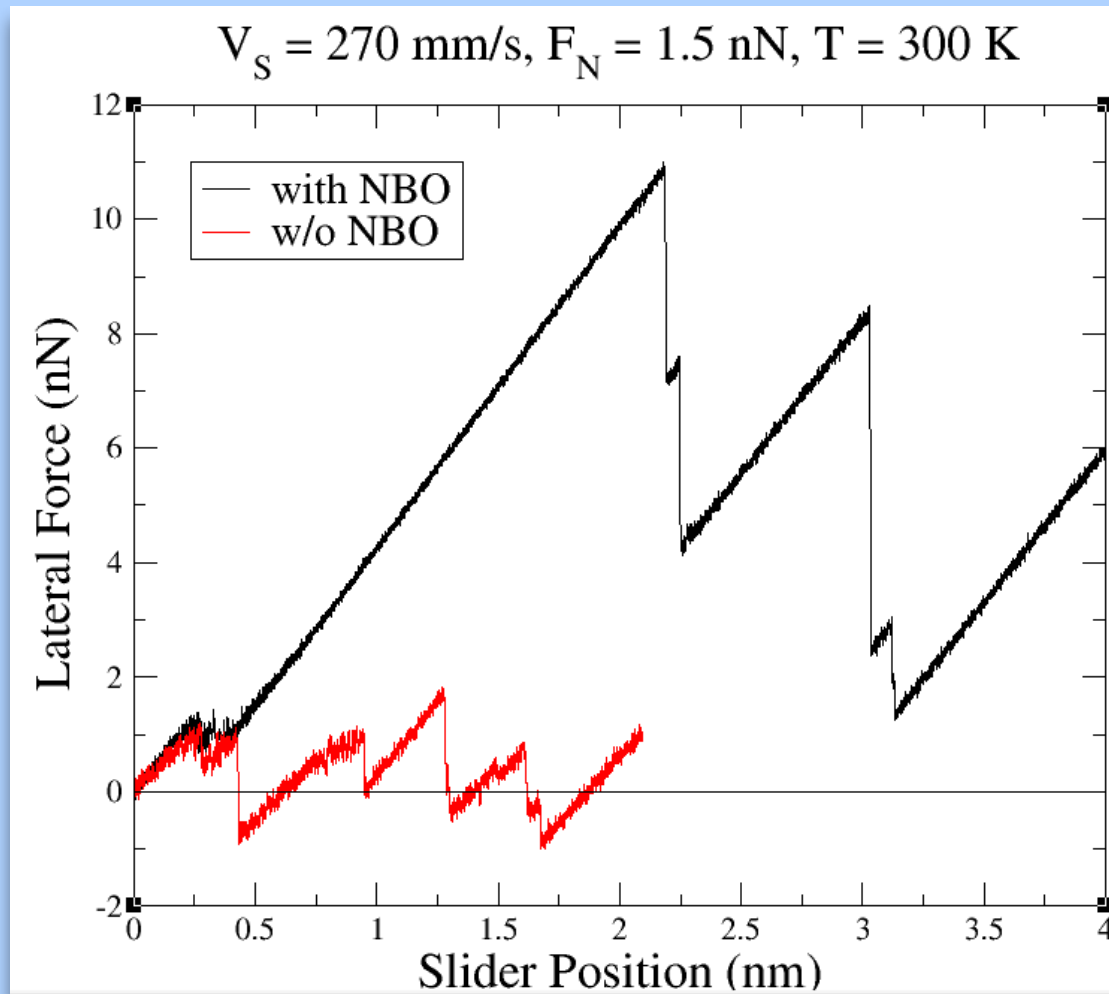
Bridging Oxygen



Non-Bridging Oxygen

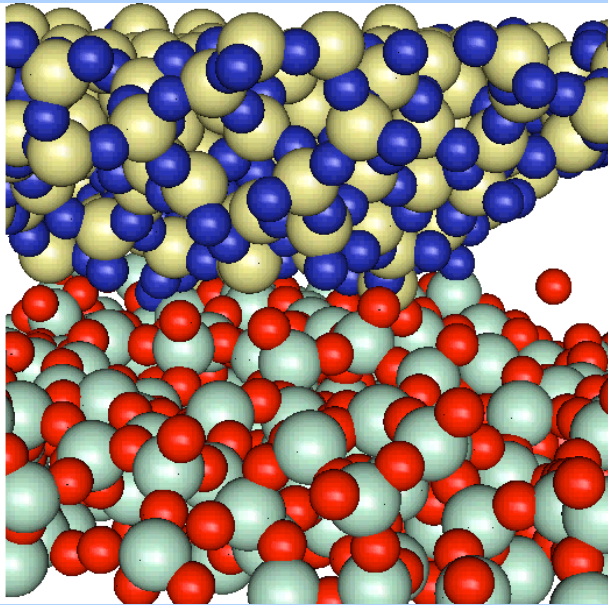


# Results From Ordinary MD

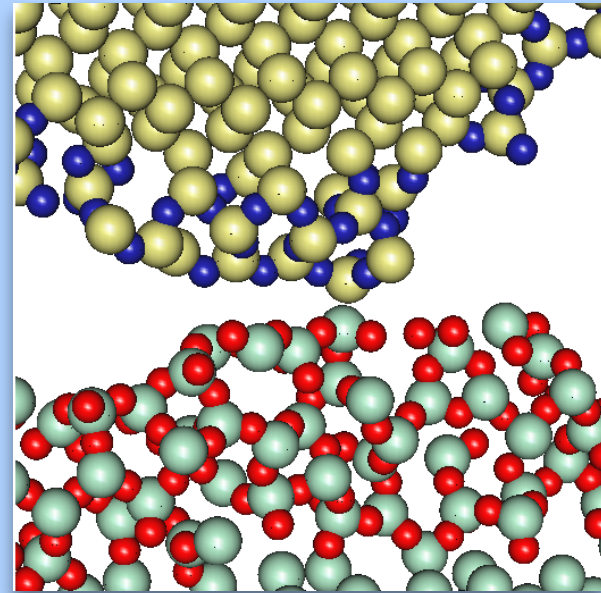


# Different Surface Chemistry

with NBO

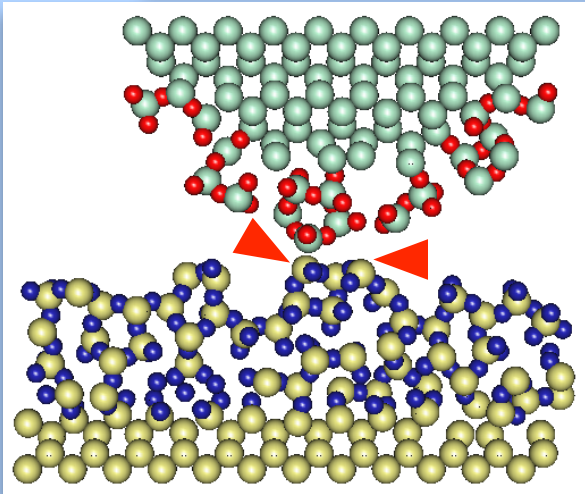
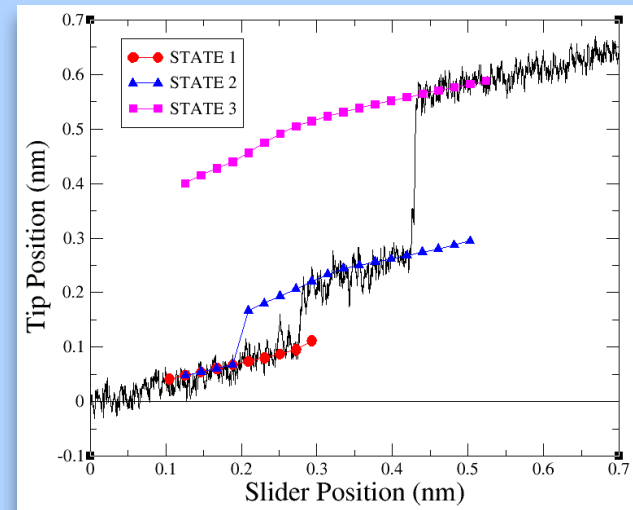
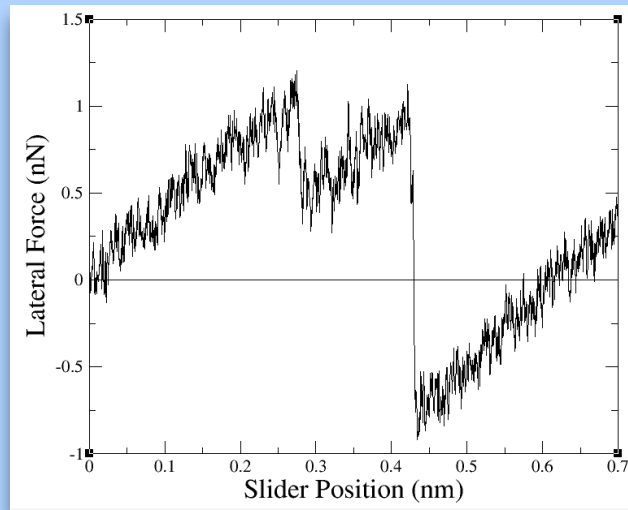


w/o NBO

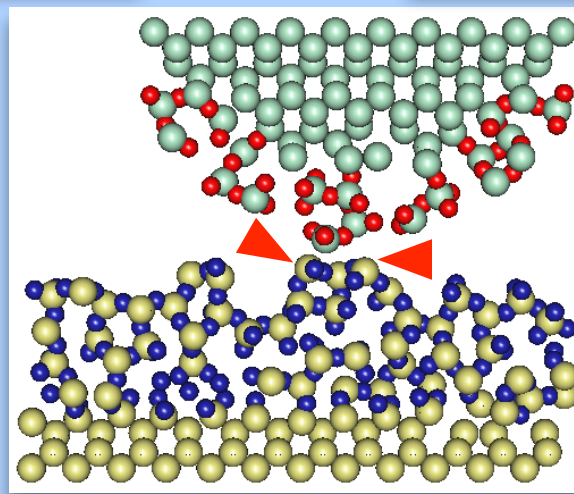


Pre-existing strong Si-O bond and  
new formation of Si-O bond

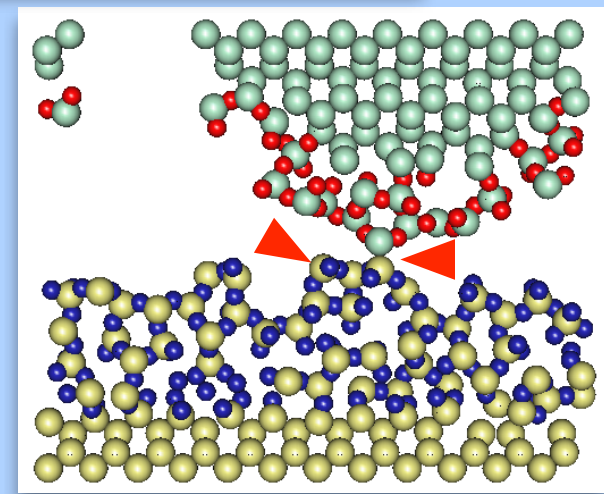
# Multistep Transitions



**STATE 1**



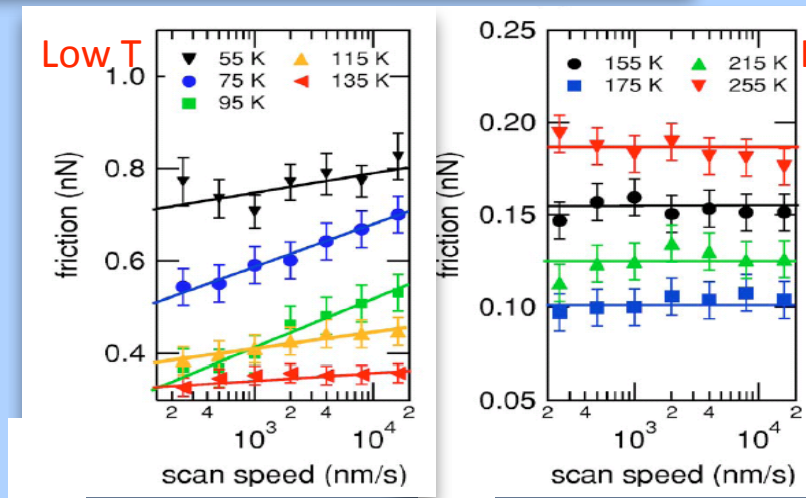
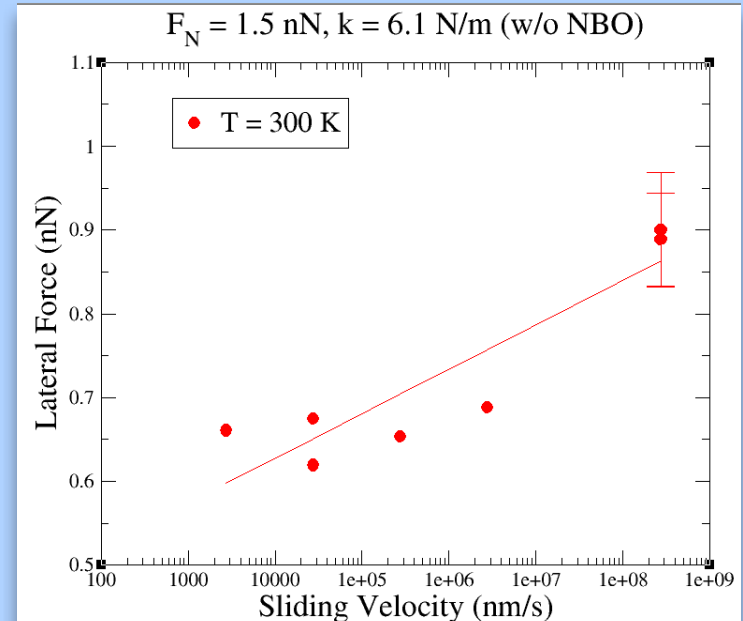
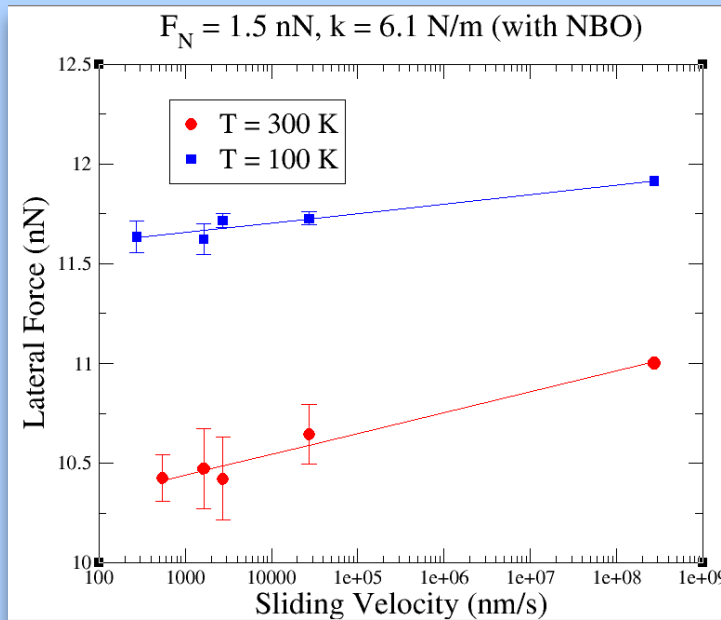
**STATE 2**



**STATE 3**

Strong evidence that the sliding behavior of amorphous surfaces cannot be described by the simple Tomlinson picture!

# Temperature and Velocity Dependence



(Schirmeisen *et al*, *Appl. Phys. Lett.*, 2006)



# Our Research Outcomes

- We have modified and extended the original hyperdynamics method for a driven system.
- The applications to the simple L-J system have validated the methodology.
- The application to the amorphous silica system shows the interesting temperature and sliding velocity dependence of friction force in both systems with NBO and without NBO.
- We achieve a **5 to 6 order of magnitude speed up** applying our boost potential to this system.

**This work was supported by the US National Science Foundation under Grants No. 0510163 and 0926111**