Montel Carlo simulation: Ising model

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Table 3.2   The quantum number n, ℓ, and m_ℓ

Principal quantum number	$n = 1, 2, 3, \ldots$
Orbital angular momentum quantum number	$\ell = 0, 1, 2, \ldots, (n-1) < n$
Magnetic quantum number	$m_\ell = -\ell, -(\ell-1), \ldots, 0, \ldots, (\ell-1), \ell$ or $|m_\ell| \leq \ell$

Table 2.1   Summary of the Relationships among the Quantum Numbers n, l, m_l and Numbers of Orbitals and Electrons

Value of n	Value of l	Values of m_l	Subshell	Number of Orbitals	Number of Electrons
1	0	0	1s	1	2
2	0	0	2s	1	2
	1	$-1, 0, +1$	2p	3	6
3	0	0	3s	1	2
	1	$-1, 0, +1$	3p	3	6
	2	$-2, -1, 0, +1, +2$	3d	5	10
4	0	0	4s	1	2
	1	$-1, 0, +1$	4p	3	6
	2	$-2, -1, 0, +1, +2$	4d	5	10
	3	$-3, -2, -1, 0, +1, +2, +3$	4f	7	14

Source: From J. E. Brady and F. Senese, *Chemistry: Matter and Its Changes,* 4th edition. Reprinted with permission of John Wiley & Sons, Inc.
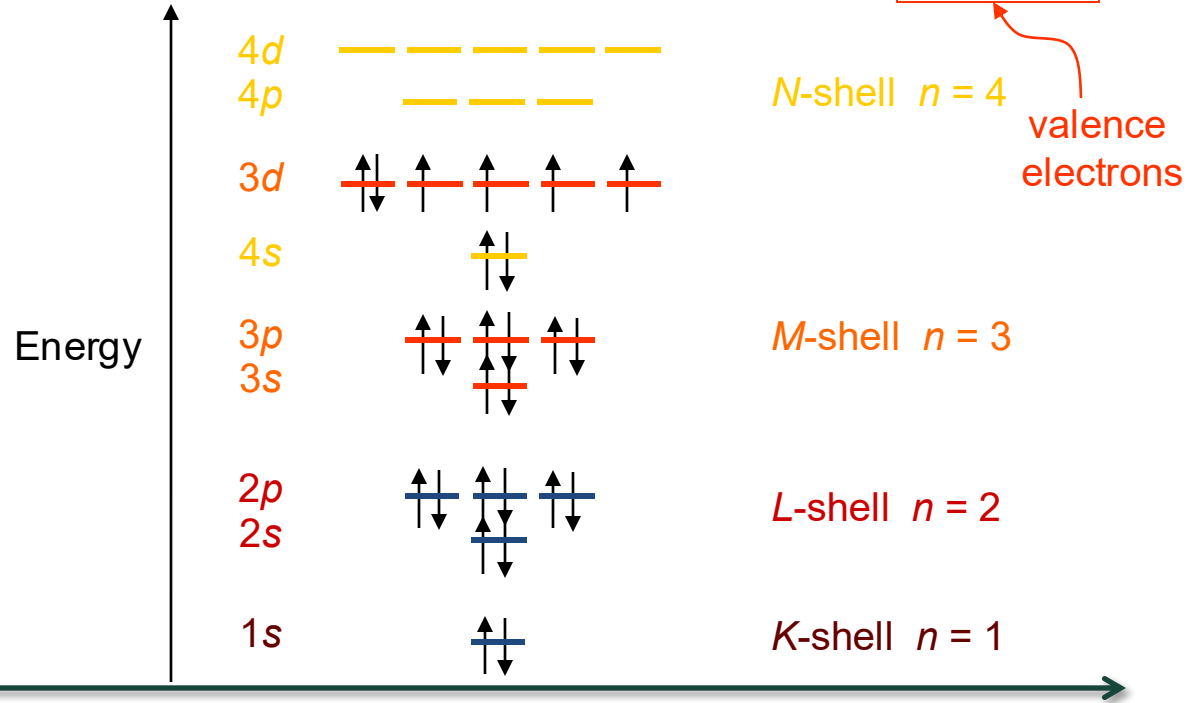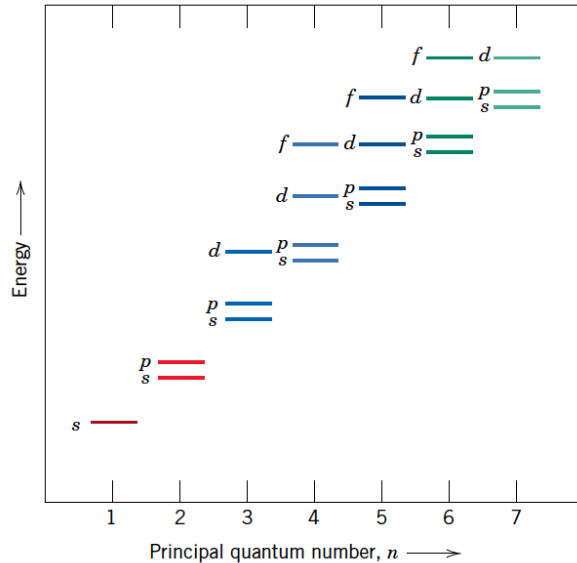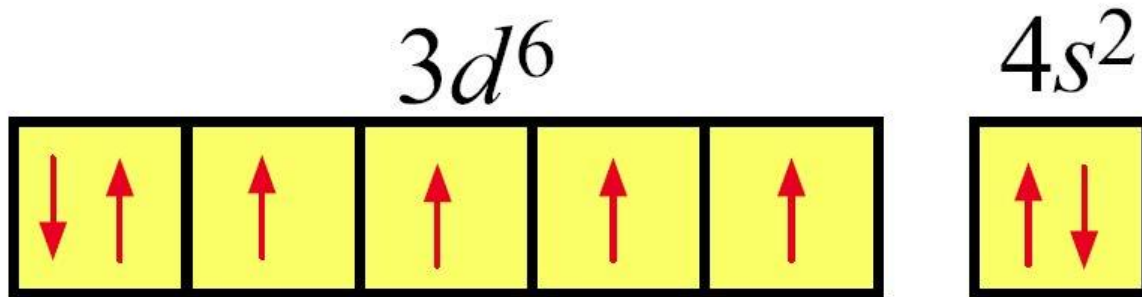
Angular equation

$$Y_{l,m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(\cos\theta) e^{im\phi}$$

$$l \geq m \quad \forall \quad m > 0$$

$$l = m \quad \text{if} \quad m = 0 \qquad \Longrightarrow \qquad l \geq |m|$$

$$l \geq -m \quad \forall \quad m < 0$$

Radial equation

$$R_{n,l}(r) = \sqrt{\left(\frac{2}{a_0 n}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}} \cdot e^{-r/a_0 n} \left(\frac{2r}{a_0 n}\right)^l \cdot L_{n-l-1}^{2l+1}\left(\frac{2r}{a_o n}\right) \qquad \Longrightarrow \qquad n - 1 > l$$

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Spin moment

$$m_s = \frac{1}{2} \text{ or } -\frac{1}{2}$$

ex: Fe - atomic # = $\quad$ 26 $\quad$ $1s^2$ $\quad$ $2s^2\,2p^6$ $\quad$ $3s^2\,3p^6$ $\quad$ $\boxed{3d^6\;\;4s^2}$

valence electrons

Level	Shell
4d	
4p	N-shell $n = 4$
3d	
4s	
3p	M-shell $n = 3$
3s	
2p	L-shell $n = 2$
2s	
1s	K-shell $n = 1$

Energy

Fe: [Ar]$3d^6 4s^2$ Electron structure

$$3d^6 \qquad\qquad 4s^2$$

- An isolated Fe atom has 4 unpaired spins and a spin magnetic moment of 4β.

Periodic Table of the Elements

Image from internet

$$\frac{M_{sat}(T)}{M_{sat}(0)}$$

Iron

Normalized saturated magnetization vs. reduced temperature T/TC where T_C is the Curie temperature (ex. 1043 K for Fe).

In Ernst Ising thesis (1924)

Total energy of the system:

$$E = -\frac{J}{2} \sum_i \sum_{j \neq i} s_i s_j - H \sum s_i$$

- There is a magnetic moment ($s_i = +1$ or -1) at each site.
- The interaction energy between two adjacent moments is $-J \cdot s_i \cdot s_j$, where J is a coefficient. Thus, if two adjacent sites have the same spin moment, the interaction energy is zero. The interaction energy is J between two sites with opposite moments.
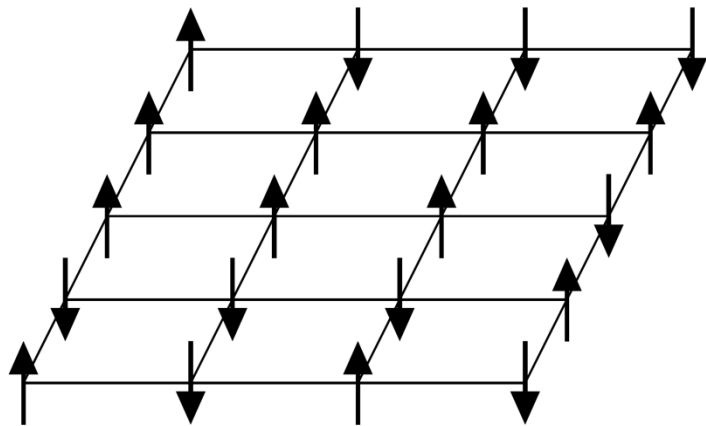- The energy resulting from the external magnetic field is $-H \cdot s_i$, i.e., aligning along the external field decreases energy.

1. Set up the initial configuration with random spins on the 2D grid system. The spins are either +1 or -1.
2. Make a random trial change: randomly select a position on the lattice and flip the spin.
3. At the selected site, compute the energy difference caused by the trial: $\Delta E_i = E_i^{tri} - E_i^{cur}$, where $E_i^{cur} = -J s_i \sum_j s_j - H s_i$ and $E_i^{tri} = -J(-s_i) \sum_j s_j - H(-s_i)$, indicates neighboring sites. Thus,
   - $\Delta E_i = 2 J s_i \sum_j s_j + 2 H s_i$.
4. Check whether the change is acceptable.
   - If $\Delta E_i \leq 0$, accept the flip.
   - If $\Delta E_i > 0$, compute the Boltzmann weighting factor $w = \exp(-\Delta E_i / kT)$. Generate a random number r. If $r < w$, accept the change. Otherwise, reject the change.
5. If the change is at the boundaries, impose boundary condition. Here, we can again use periodic boundary conditions.
6. Repeat the sampling procedure (2--5)
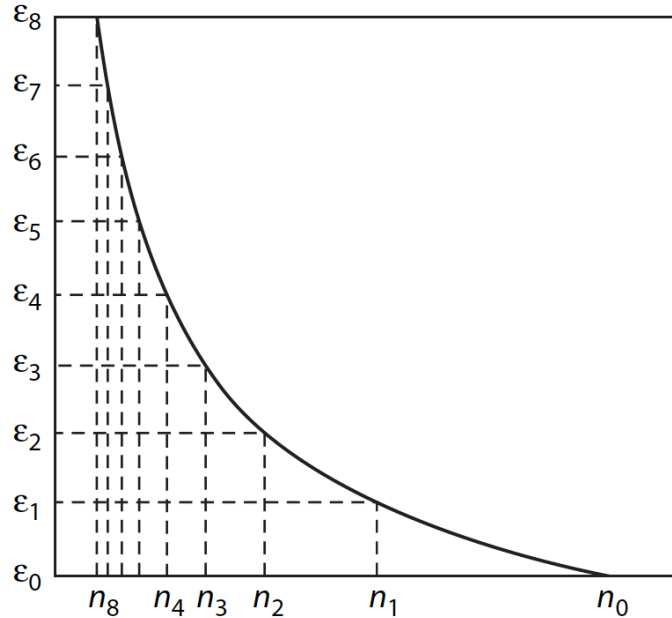
$$\Omega = \frac{N!}{n! \cdot (N-n)!}$$

Boltzmann distribution
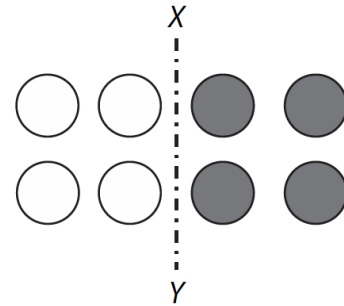
Combinatorial configuration

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Number of configuration of the system

$$\Omega = \frac{n!}{n_0! \, n_1! \, n_2! \, \ldots \, n_r!}$$

Stirling approximation: $\ln X! = X \ln X - X$

$$\ln \Omega = n \ln n - n - \Sigma(n_i \ln n_i - n_i)$$

$$\delta \ln \Omega = -\Sigma \delta n_i \ln n_i \rightarrow \delta \ln \Omega = -\Sigma \delta n_i \ln n_i = 0$$

$$\Sigma(\ln n_i + \alpha + \beta \varepsilon_i)\delta n_i = 0 \rightarrow \ln n_i = -\alpha - \beta \varepsilon_i$$

$$n_i = e^{-\alpha}e^{-\beta \varepsilon_i} \qquad n = e^{-\alpha}\Sigma e^{-\beta \varepsilon_i} \rightarrow e^{-\alpha} = \frac{n}{\Sigma e^{-\beta \varepsilon_i}} = \frac{n}{Z}$$

- n_i: the number of atoms at energy state ε_i
- $n = \Sigma n_i$
- $U = \Sigma n_i \varepsilon_i$
- $\delta n = \Sigma \delta n_i = 0 \rightarrow \Sigma \alpha \delta n_i = 0$
- $\delta U = \Sigma \varepsilon_i \delta n_i = 0 \rightarrow \Sigma \beta \varepsilon_i \delta n_i = 0$

- k_B: 1.38065×10^{-23} J/K
- $R = k_B N_0$

Boltzmann distribution $\quad n_i = \dfrac{ne^{-\beta \varepsilon_i}}{Z}$

Boltzmann constant $\quad \beta = \dfrac{1}{k_B T}$

Partition function $\quad Z = \Sigma e^{-\frac{\varepsilon_i}{k_B T}}$

12

DYNAMIC MODELS OF SEGREGATION†

THOMAS C. SCHELLING
Harvard University

Some segregation results from the practices of organizations, some from specialized communication systems, some from correlation with a variable that is non-random; and some results from the interplay of individual choices. This is an abstract study of the interactive dynamics of discriminatory individual choices. One model is a simulation in which individual members of two recognizable groups distribute themselves in neighborhoods defined by reference to their own locations. A second model is analytic and deals with compartmented space. A final section applies the analytics to 'neighborhood tipping.' The systemic effects are found to be overwhelming: there is no simple correspondence of individual incentive to collective results. Exaggerated separation and patterning result from the dynamics of movement. Inferences about individual motives can usually not be drawn from aggregate patterns. Some unexpected phenomena, like density and vacancy, are generated. A general theory of 'tipping' begins to emerge.
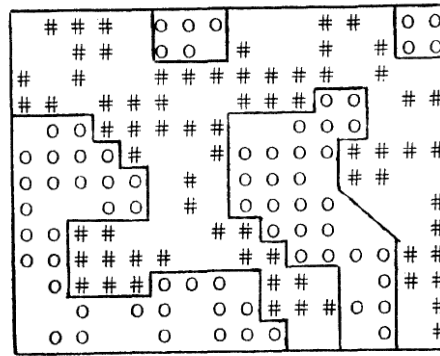
Schelling was awarded the 2005 Nobel Memorial Prize in Economic Sciences (shared with Robert Aumann) for "having enhanced our understanding of conflict and cooperation through game theory analysis." wikipedia
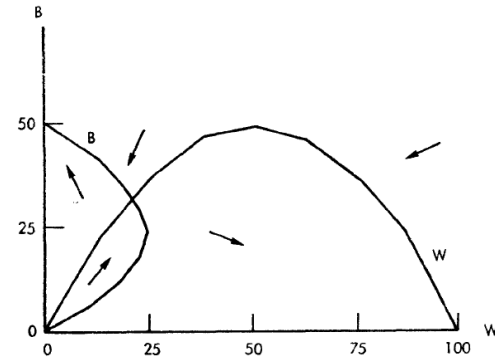

Fig. 10

Fig. 18

Racial segregation map based on USA Census 2020

https://www.arcgis.com/apps/mapviewer/index.html?webmap=30d2e10d4d694b3eb4dc4d2e58dbb5a5

- Regular Monte Carlo is good for estimate equilibrium quantities.
  - No physical time unit is associated with sampling.
- Kinetic Monte Carlo adds one more feature: each sampling event is associated with rate of event occurrence. Thus, when a sampling even is proceeded, the time advances with dt.
- Application: calculate diffusion coefficient.

$$D_J = \lim_{t \to \infty} \frac{1}{4t} \frac{1}{N} \left\langle \left(\Sigma_i^N \vec{r}_i \right)^2 \right\rangle$$

- Example: calculating lithium diffusivity using kinetic Monte Carlo

Anton Van der Ven

Associate Chair
Professor, Materials

Faculty Website

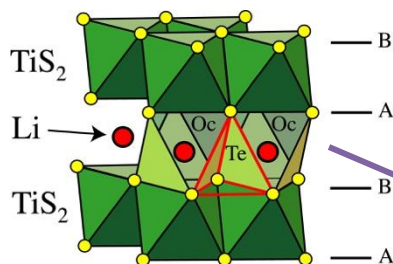Contact
(805) 893-7920
avdv@engineering.ucsb.edu

1361A Engineering II
University of California, Santa Barbara
Santa Barbara, CA 93106-5050

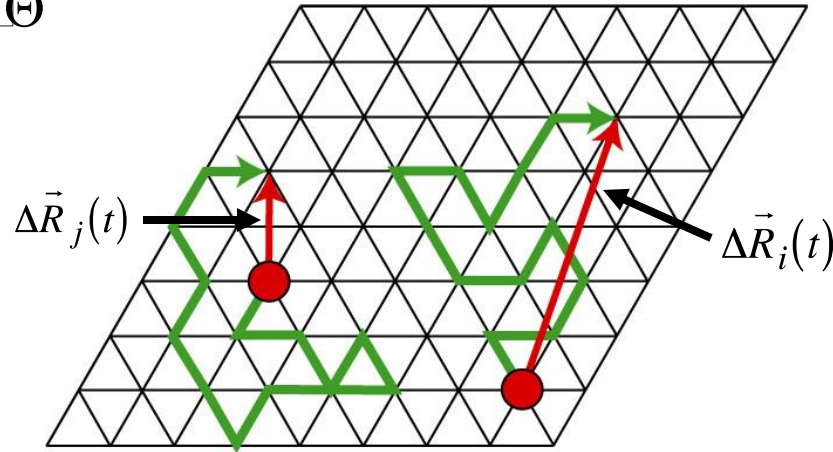**Lithium-vacancy disorder over interstitial sites**

Assign occupation variables to each position in crystal

$$\sigma_i = +1 \quad \text{if atom \textbf{Lithium} occupies site } i$$

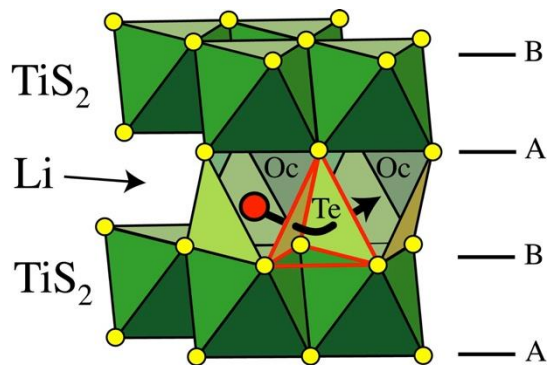$$\sigma_i = -1 \quad \text{if atom \textbf{Vacancy} occupies site } i$$
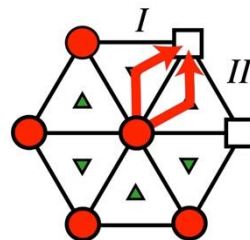
$$D = D_J \times \widetilde{\Theta}$$

$$\Delta \vec{R}_j(t)$$
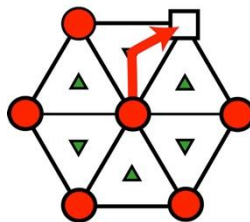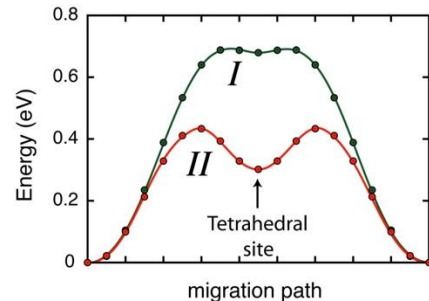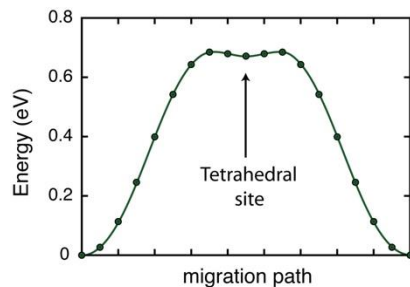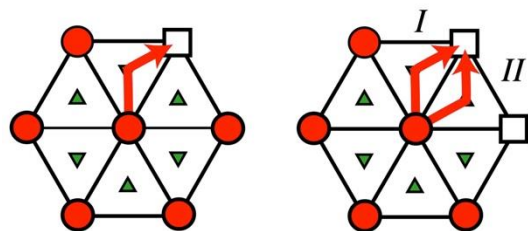
$$\Delta \vec{R}_i(t)$$
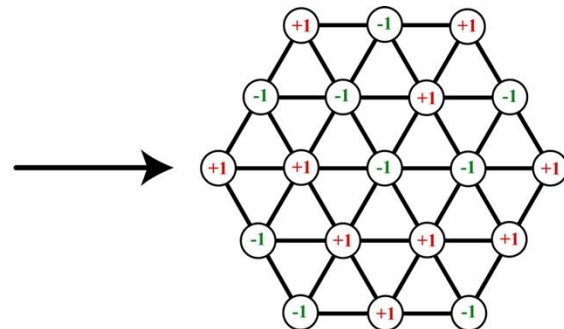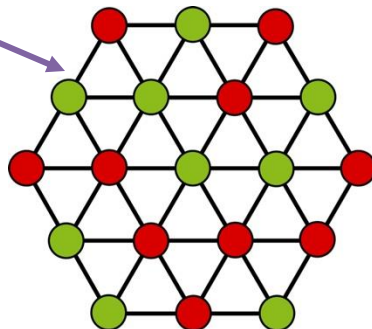
self-diffusivity $$D_J = \frac{1}{(2d)t} \left\langle \frac{1}{N} \left(\sum_{i=1}^{N} \Delta \vec{R}_i(t) \right)^2 \right\rangle$$
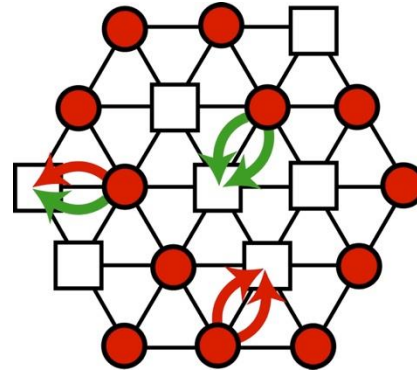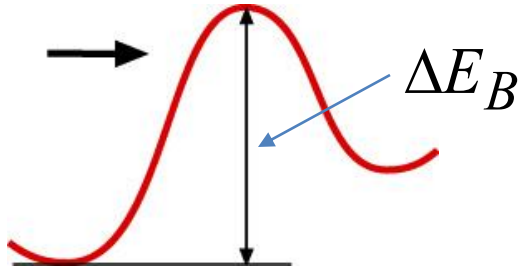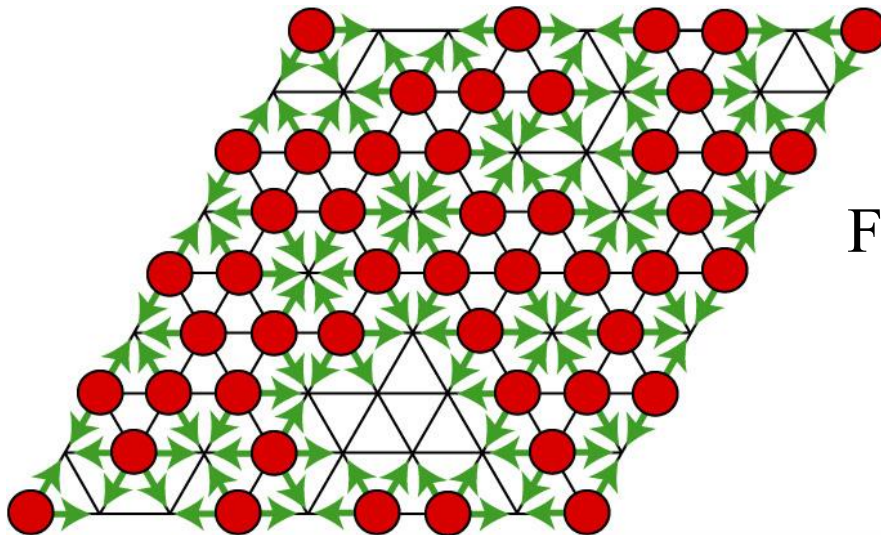
Dependence on local environment

Short-time coarse graining:
Reduce rare-event hops to a hop frequency

$$\Gamma = \nu * \exp\left(\frac{-\Delta E_B}{kT}\right)$$

$$\nu* = \frac{\overset{3N}{\underset{i}{\prod}} \nu_i^{initial}}{\overset{3N-1}{\underset{j}{\prod}} \nu_j^{activated}}$$

ΔE_B

Vineyard, J. Phys. Chem. Solids **3**, 121 (1957).

For each potential hop i, calculate the hop rate

$$W_i = \nu * \exp\left(\frac{-\Delta E_i}{k_B T}\right)$$
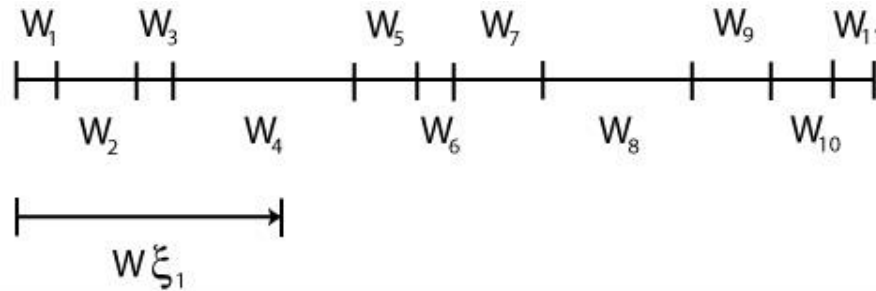
Then randomly choose a hop k, with probability W_k

$\xi_1 =$ random number

Randomly choose a hop k, with probability W_k

$$\xi_1 = \text{random number}$$

$$\sum_{i=1}^{k-1} W_i < \xi_1 \times W \leq \sum_{i=0}^{k} W_i \qquad\qquad W = \sum_{i=0}^{N_{hops}} W_i$$

Diffusion coefficients

$$D = D_J \times \widetilde{\Theta}$$
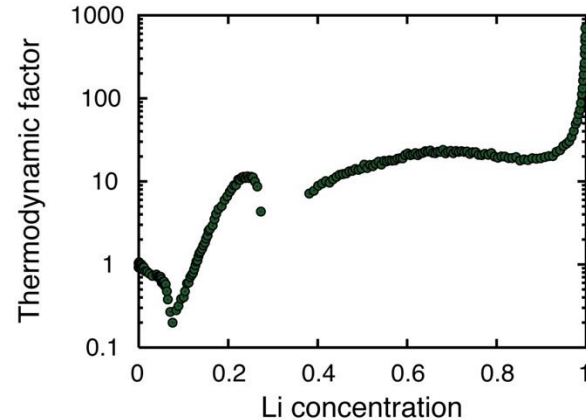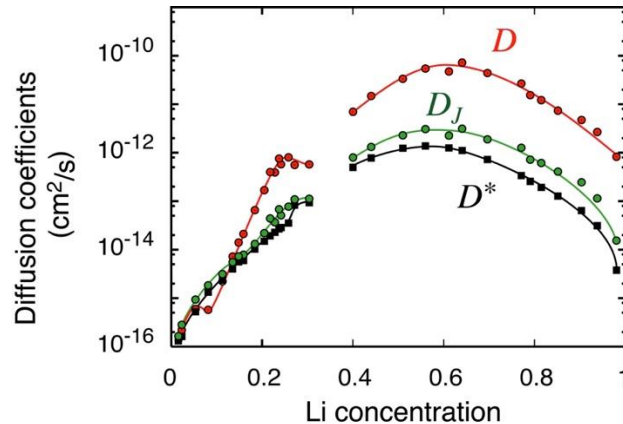
$$D_J = \frac{1}{(2d)t} \left\langle \frac{1}{N} \left(\sum_{i=1}^{N} \Delta \vec{R}_i(t) \right)^2 \right\rangle$$

$$\widetilde{\Theta} = \frac{\partial \left(\frac{\mu_{Li}}{kT} \right)}{\partial \ln x_{Li}}$$

A. Van der Ven, J. C. Thomas, Q. Xu, B. Swoboda, D. Morgan, Phys. Rev. B, vol 78, 104306 (2008)