

Montel Carlo simulation: Ising model

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Table 3.2 The quantum number n , ℓ , and m_ℓ

Principal quantum number	$n = 1, 2, 3, \dots$
Orbital angular momentum quantum number	$\ell = 0, 1, 2, \dots, (n - 1) < n$
Magnetic quantum number	$m_\ell = -\ell, -(\ell - 1), \dots, 0, \dots, (\ell - 1), \ell$ 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
	0	0	4s	1	2
4	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

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

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

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

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

Radial equation

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



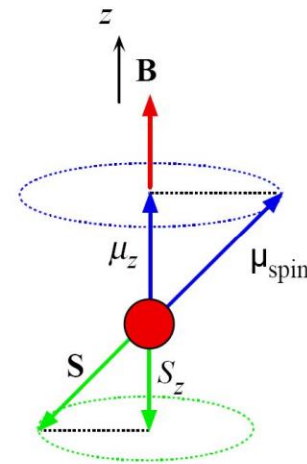
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	3	-3, -2, -1, 0, +1, +2, +3	4f	7	14

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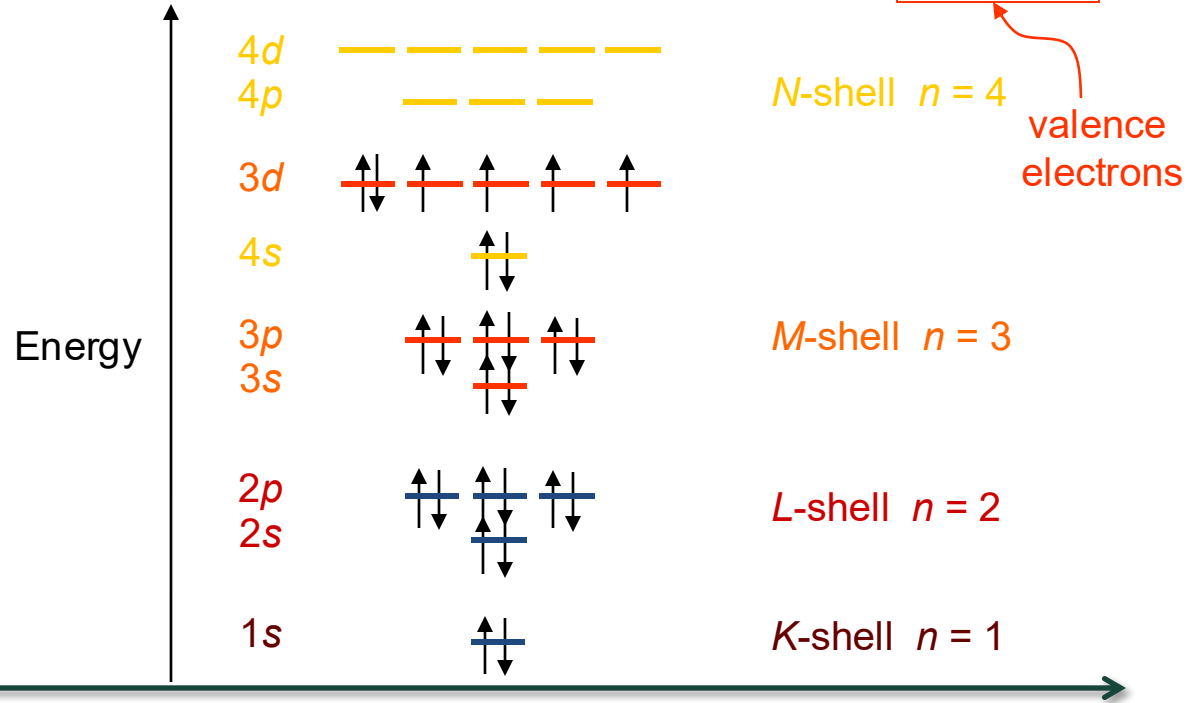
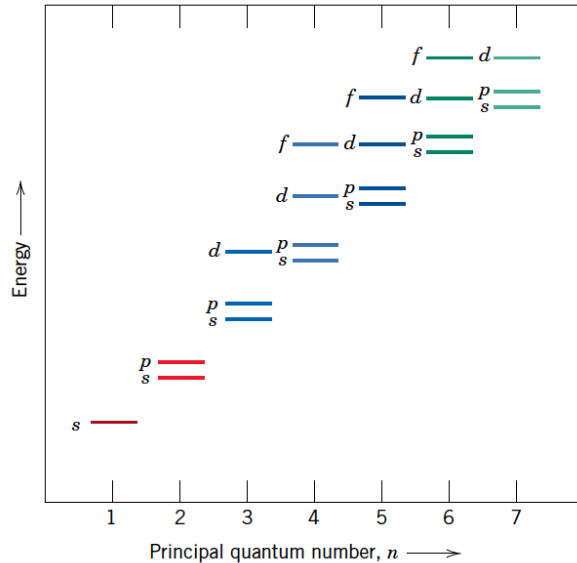


Spin moment

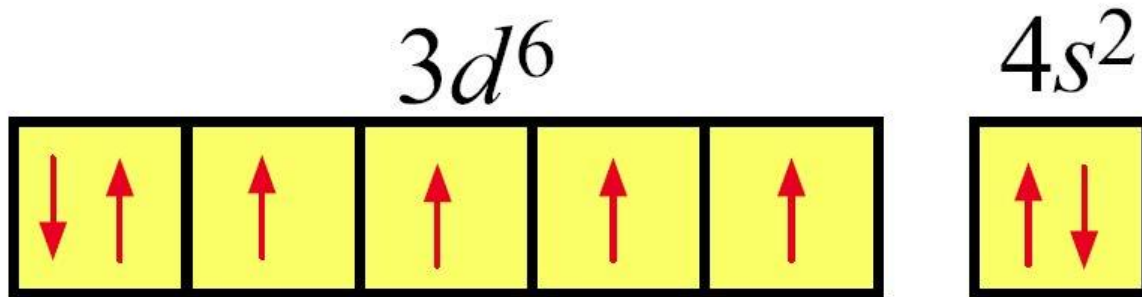
$$m_s = \frac{1}{2} \text{ or } -\frac{1}{2}$$



ex: Fe - atomic # = 26 $1s^2 2s^2 2p^6 3s^2 3p^6$ $3d^6 4s^2$



Fe: $[\text{Ar}]3d^64s^2$ Electron structure



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



Elements with ferromagnetisms

Periodic Table of the Elements

Group 1

Period 1

1.008
1
H
Hydrogen

2

3 4

6.94
3
Li
Lithium

9.0122
4
Be
Beryllium

22.990
11
Na
Sodium

24.305
12
Mg
Magnesium

39.098
19
K
Potassium

40.078
20
Ca
Calcium

85.468
37
Rb
Rubidium

87.62
38
Sr
Strontium

132.91
55
Cs
Cesium

137.33
56
Ba
Barium

223
87
Fr
Francium

226
88
Ra
Radium

standard atomic weight
or most stable mass number

1st ionization energy
in kJ/mol

chemical symbol

name

electron configuration

radioactive elements have
masses in parenthesis

55.845
26
Fe
Iron
[Ar] 3d⁶ 4s²

atomic number

electronegativity

oxidation states
most common are bold

13 14 15 16 17 18

10.81
5
B
Boron

12.011
6
C
Carbon

14.007
7
N
Nitrogen

15.999
8
O
Oxygen

18.998
9
F
Fluorine

20.180
10
Ne
Neon

26.982
13
Al
Aluminum

28.085
14
Si
Silicon

30.974
15
P
Phosphorus

32.06
16
S
Sulfur

35.45
17
Cl
Chlorine

39.948
18
Ar
Argon

69.723
31
Ga
Gallium

72.630
32
Ge
Germanium

74.922
33
As
Arsenic

78.971
34
Se
Selenium

79.904
35
Br
Bromine

83.798
36
Kr
Krypton

114.82
49
In
Indium

118.71
50
Sn
Tin

121.76
51
Sb
Antimony

127.60
52
Te
Tellurium

126.90
53
I
Iodine

131.29
54
Xe
Xenon

175.07
81
Tl
Thallium

175.94
82
Pb
Lead

183.84
83
Bi
Bismuth

186.21
84
Po
Polonium

188.906
85
At
Astatine

189.122
86
Rn
Radon

208.98
83
Tl
Thallium

207.2
82
Pb
Lead

208.98
83
Bi
Bismuth

209
84
Po
Polonium

209
85
At
Astatine

209
86
Rn
Radon

223
87
Fr
Francium

226
88
Ra
Radium

227
89
Ac
Actinium

232.04
90
Th
Thorium

231.04
91
Pa
Protactinium

238.03
92
U
Uranium

237
93
Np
Neptunium

244
94
Pu
Plutonium

247
95
Am
Americium

251
96
Cm
Curium

252
97
Bk
Berkelium

257
98
Cf
Californium

259
99
Es
Einsteinium

262
100
Fm
Fermium

267
101
Md
Mendelevium

271
102
No
Nobelium

Electron configuration blocks

s d p

f

Notes

- 1 kJ/mol = 0.0103636 eV
- all elements are implied to have an oxidation state of zero

by Robert Campbell - updated 2016, 2018

3 4 5 6 7 8 9 10 11 12

44.956
21
Sc
Scandium

47.867
22
Ti
Titanium

50.942
23
V
Vanadium

51.996
24
Cr
Chromium

54.938
25
Mn
Manganese

58.933
26
Fe
Iron

58.933
27
Co
Cobalt

58.933
28
Ni
Nickel

63.546
29
Cu
Copper

65.38
30
Zn
Zinc

69.723
31
Ga
Gallium

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32
Ge
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Arsenic

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Selenium

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Br
Bromine

83.798
36
Kr
Krypton

88.906
39
Y
Yttrium

91.224
40
Zr
Zirconium

92.906
41
Nb
Niobium

95.95
42
Mo
Molybdenum

98
43
Tc
Technetium

101.07
44
Ru
Ruthenium

101.07
45
Rh
Rhodium

106.42
46
Pd
Palladium

107.87
47
Ag
Silver

112.41
48
Cd
Cadmium

114.82
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In
Indium

118.71
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257
98
Cf
Californium

259
99
Es
Einsteinium

262
100
Fm
Fermium

267
101
Md
Mendelevium

271
102
No
Nobelium

alkali metals

alkaline earth metals

lanthanides

actinides

transition metals

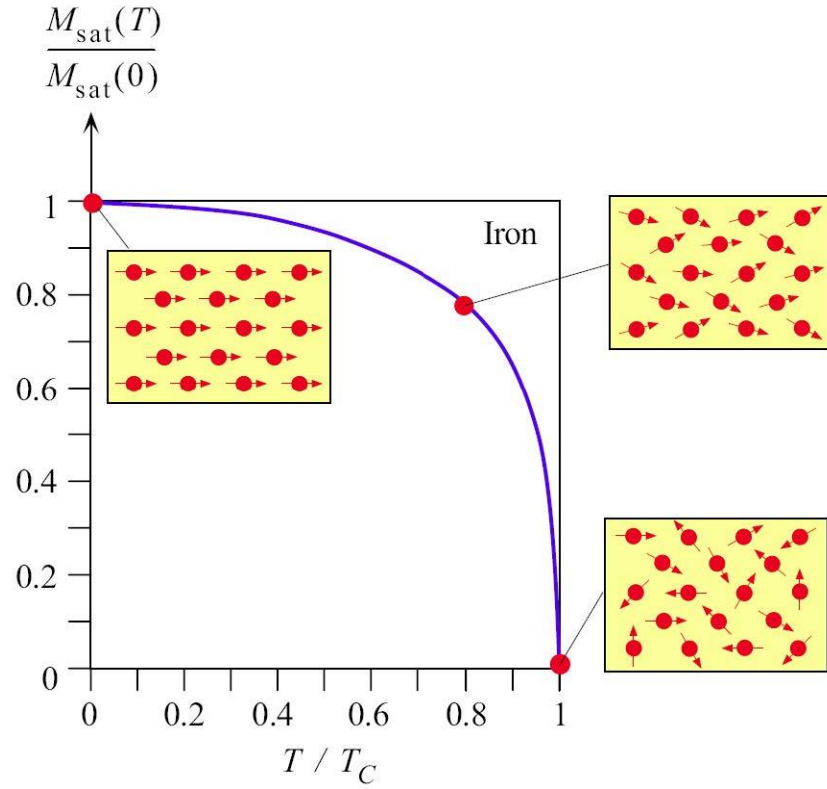
unknown properties

post-transition metals

metalloids

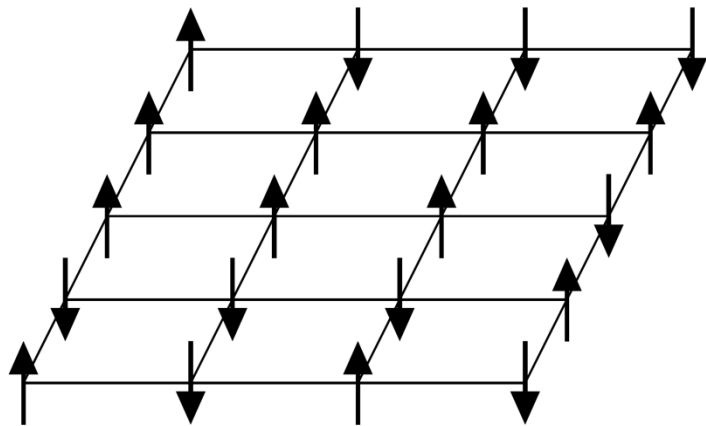
reactive nonmetals

noble gases



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

In Ernst Ising thesis (1924)



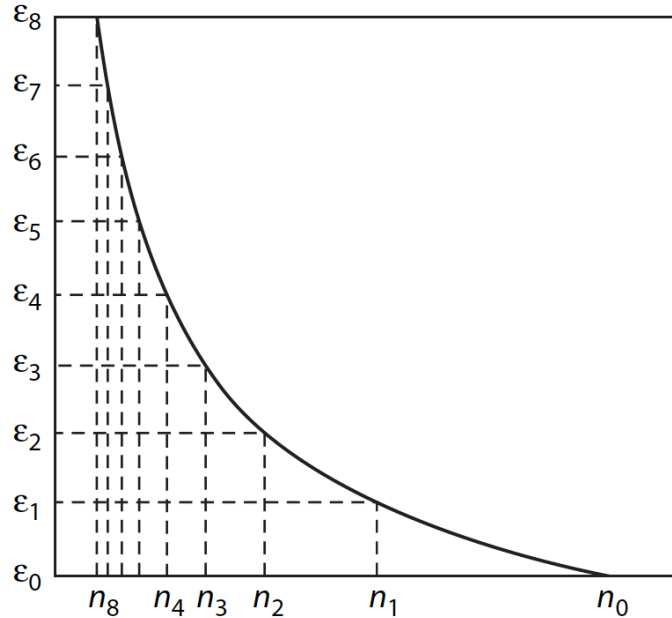
Total energy of the system:

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

- 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.

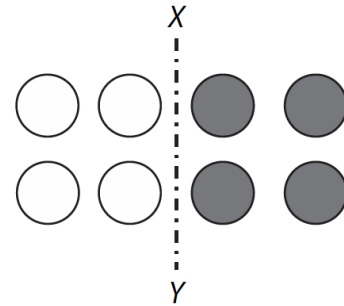
1. Set up the initial configuration with random spins on the 2D grid system. The spins are either +1 or -1.
2. Make a random trial change: randomly select a position on the lattice and flip the spin.
3. At the selected site, compute the energy difference caused by the trial: $\Delta E_i = E_i^{tri} - E_i^{cur}$, 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,
 - $\Delta E_i = 2J s_i \sum_j s_j + 2H s_i$.
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)





Boltzmann distribution

$$\Omega = \frac{N!}{n! \cdot (N - n)!}$$



Combinatorial configuration



Number of configuration of the system

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

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

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

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

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

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

Boltzmann
distribution

$$n_i = \frac{n e^{-\beta \varepsilon_i}}{Z}$$

Boltzmann
constant

$$\beta = \frac{1}{k_B T}$$

Partition
function

$$Z = \sum e^{-\frac{\varepsilon_i}{k_B T}}$$

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

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

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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.

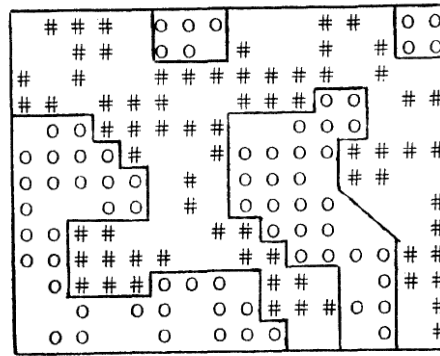


Fig. 10

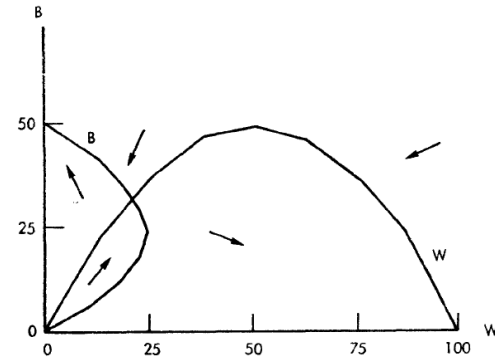


Fig. 18

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.

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

- Example: calculating lithium diffusivity using kinetic Monte Carlo



Anton Van der Ven



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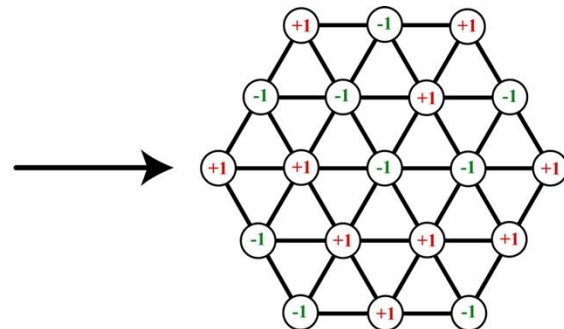
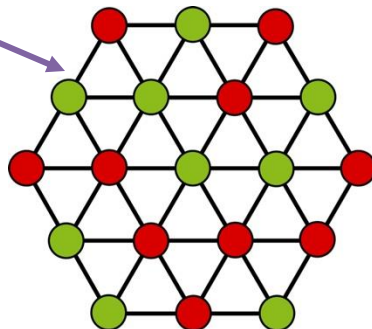
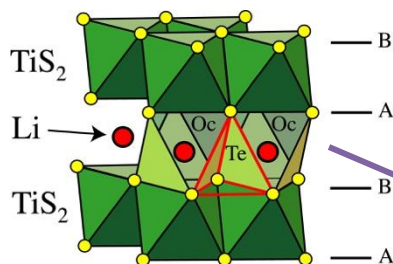
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Lithium-vacancy disorder over interstitial sites

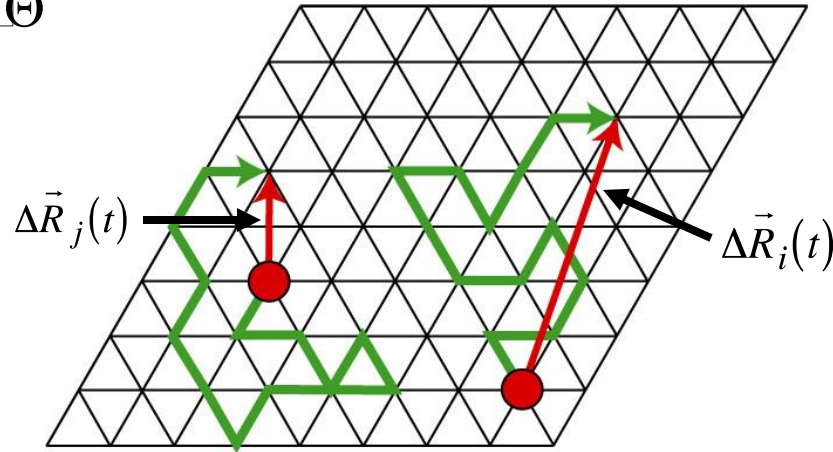
Assign occupation variables to each position in crystal

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

$$\sigma_i = -1 \quad \text{if atom \textbf{Vacancy} occupies site } i$$



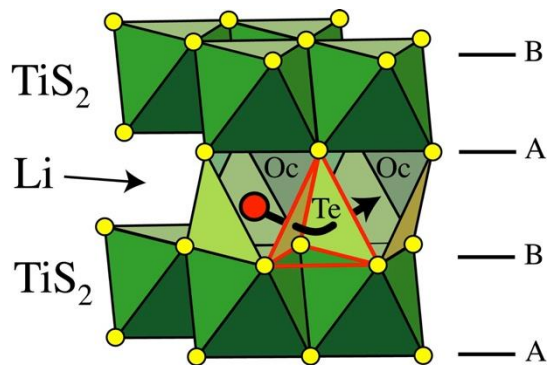
$$D = D_J \square \tilde{\Theta}$$



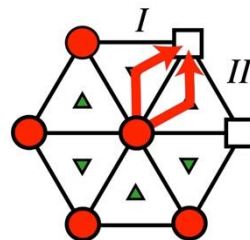
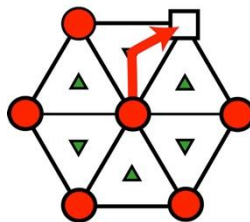
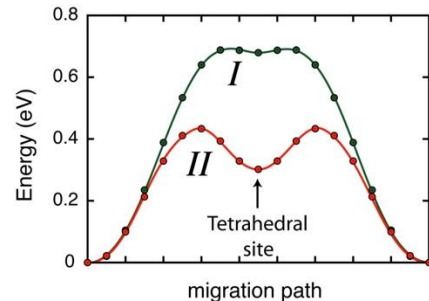
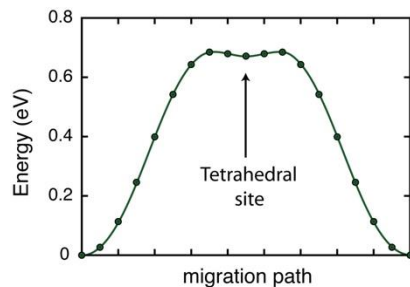
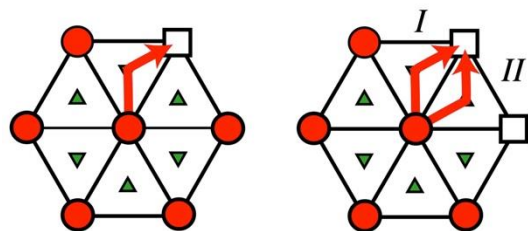
self-diffusivity

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





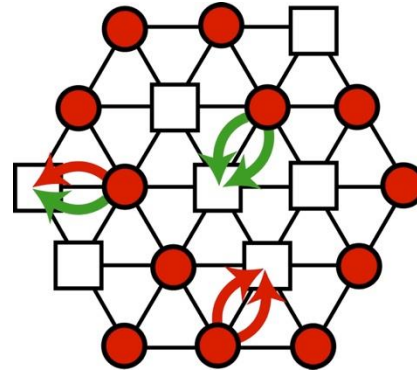
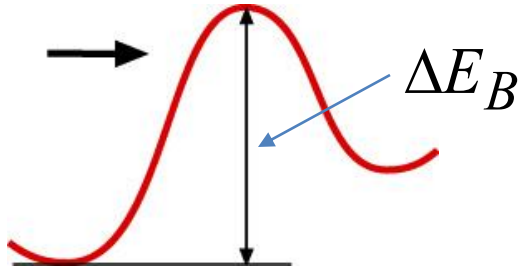
Dependence on local environment



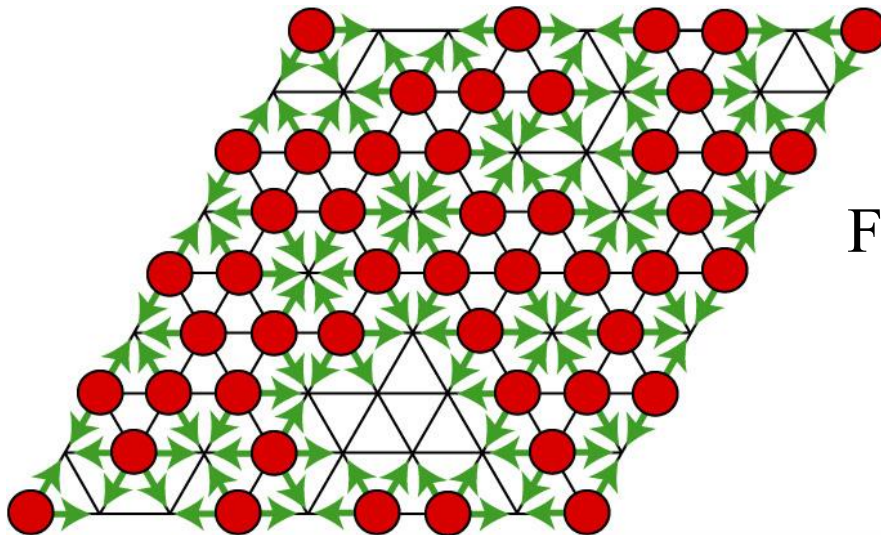
Short-time coarse graining: Reduce rare-event hops to a hop frequency

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

$$\nu^* = \frac{\frac{1}{3N} \sum_i \nu_i^{initial}}{\frac{1}{3N-1} \sum_j \nu_j^{activated}}$$



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



For each potential hop i ,
calculate the hop rate

$$W_i = v * \exp\left(\frac{-\Delta E_i}{k_B T}\right)$$

Then randomly choose a hop k , with probability W_k

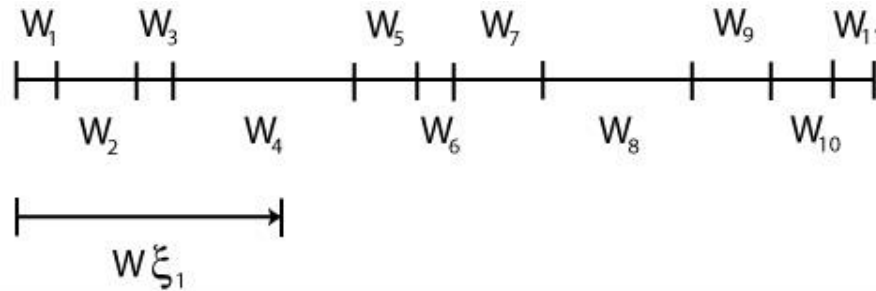
ξ_1 = random number

Randomly choose a hop k , with probability W_k

ξ_1 = random number

$$\prod_{i=1}^{k-1} W_i < \xi_1 \leq \prod_{i=0}^k W_i$$

$$W = \prod_{i=0}^{N_{hops}} W_i$$

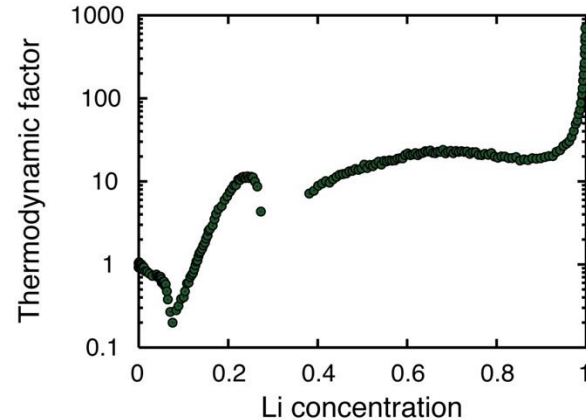
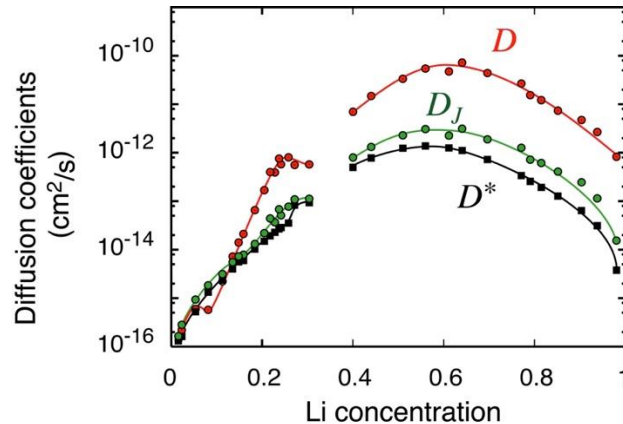


Diffusion coefficients

$$D = D_J \Theta$$

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

$$\Theta = \frac{\frac{\mu_{Li}}{kT}}{\ln x_{Li}}$$



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