Synthesis of Electrode Materials
IX International School-Conference of Young Scientists 2024

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Introduction to Atomistic Modeling: Connection to Materials Synthesis

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Computational track chronology at ICYS series

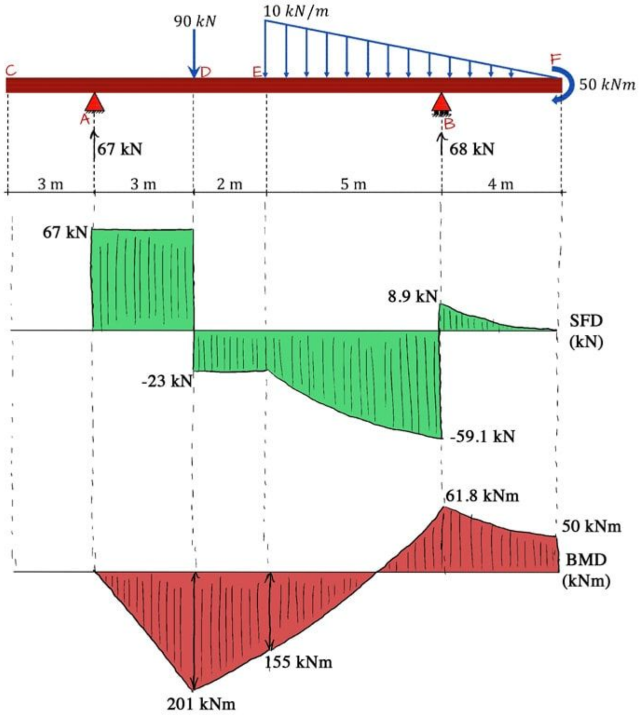
- 2021 ICYS VI *Solid State Chemistry of Battery Materials*
    - Computational track: Modeling of Intercalation potential, Li-ion diffusion in solid electrolyte
- 2022 ICYS VII *Electrochemical Materials Science*
    - Computational track: Modeling of transition metals and ligands impact on Na-ion potential and diffusion
- 2023 ICYS VIII *Crystallography of Energy Materials*
    - Computational track: Modelling of point defects energetics and diffusion
- 2024 ICYS VIII *Synthesis of Electrode Materials (!)*
    - Computational track: Calculate solubility in solids, Calculate phase diagrams, Predict morphology of particles, Calculate XAS spectra

Plan of lecture

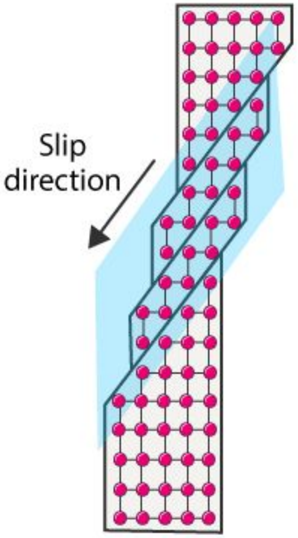
- Short introduction to materials modeling
- How to model/approach co-precipitation synthesis of cathode material?
- Basics of quantum level atomistic modeling (DFT)

Modeling of solids

Strength of materials (elastic) - continuum models based on Hooke's law

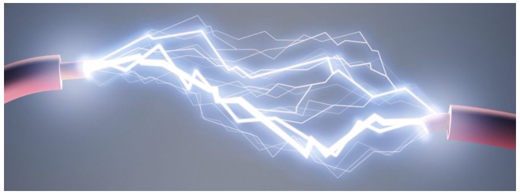


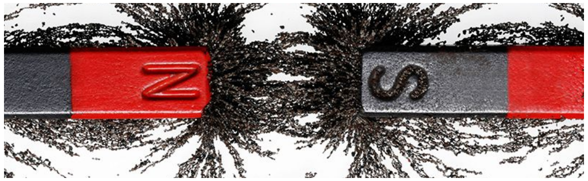
Plastic deformation? - atomic level is required

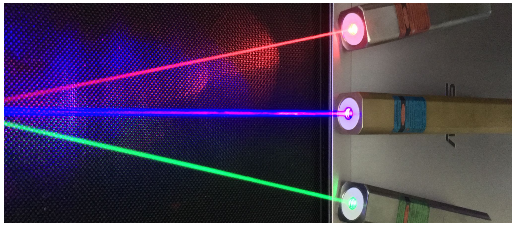


(a) Slip

Functional properties? electronic level is required

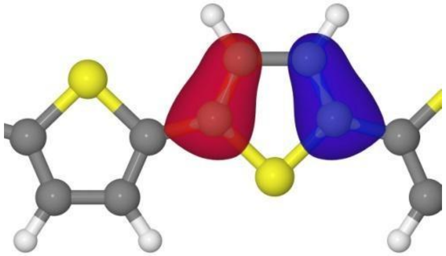


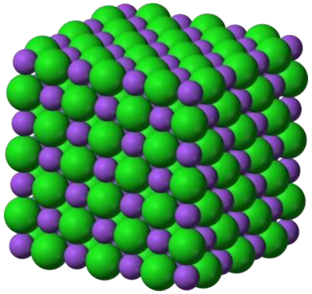




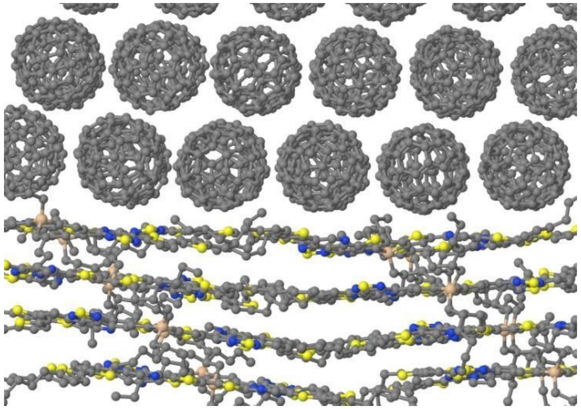
- Atomistic modeling is essentially required for detailed understanding of functional materials
- Only atomistic modeling can help to predict new materials

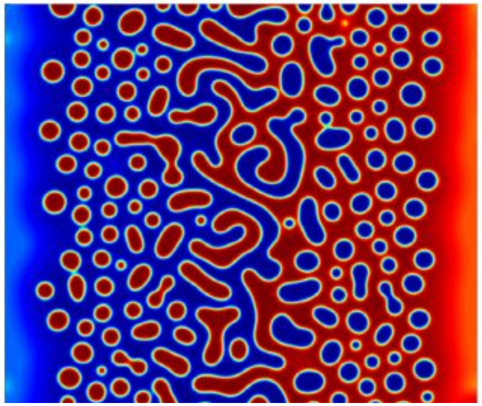
Methods vs scales



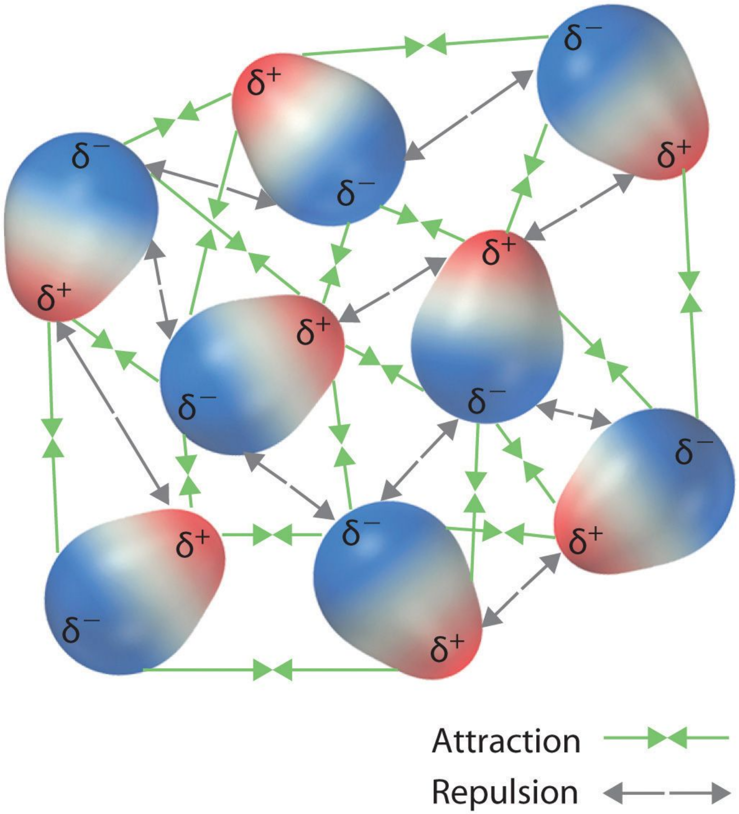


- $<10^{2-5}$ atoms, <10nm, <100 ps
    - Density Functional Theory
    - (post) Hartree-Fock
    - Semiempirical
- $< 10^{9}$ atoms, <1 µm, <100 ns
    - Parametrized
    - Classical, Machine Learned)
    - QM/MM
- Not atomistic Meso, <1mm, <1 hour
    - Kinetic Monte-Carlo
    - Phase-field models
- Not atomistic Macro, ~1m, ~ms-days
    - Finite elements
    - continuum models (diff. eq.)

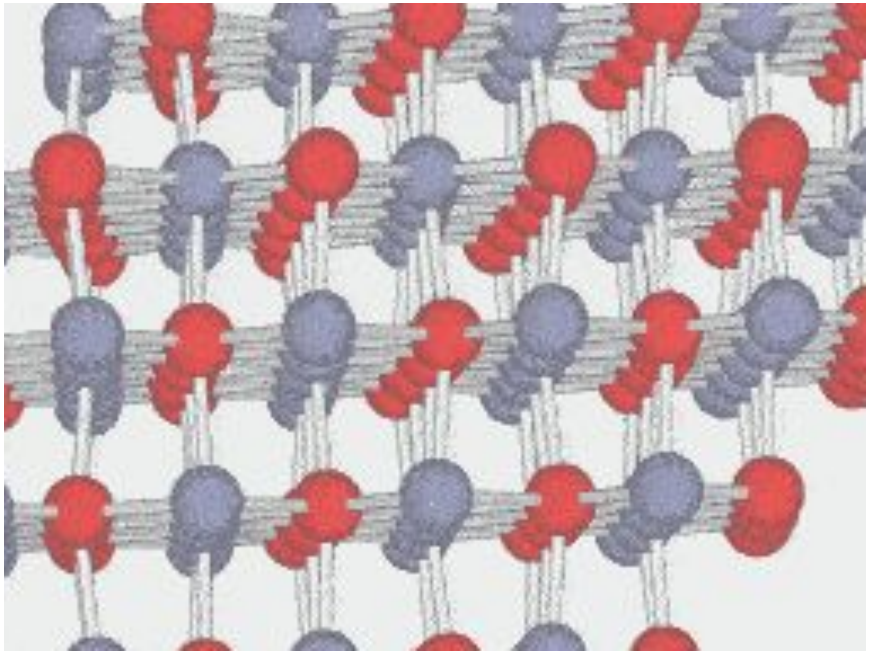




Description on atomistic level: interaction + dynamics



F = dE/dx

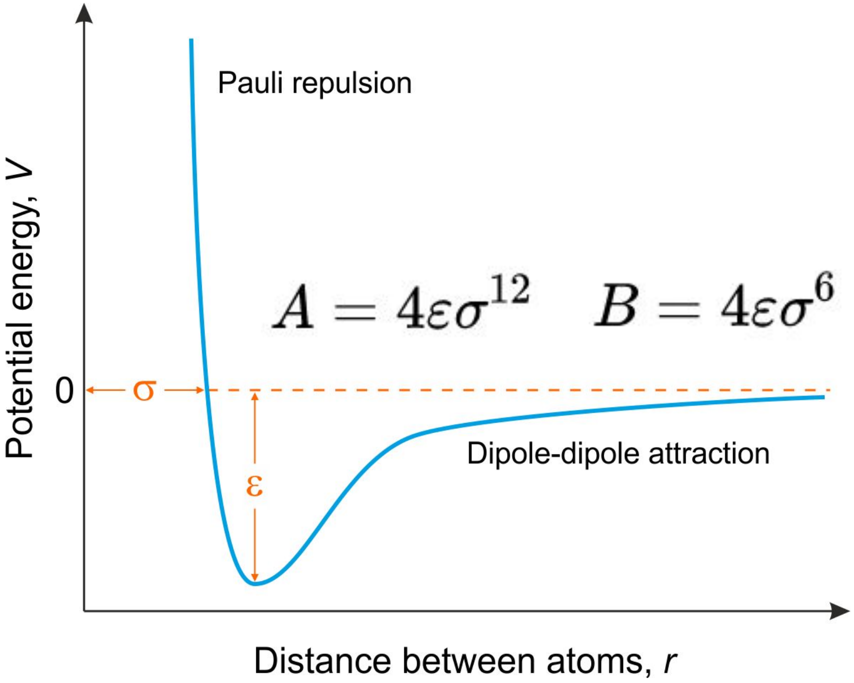


Interaction between atoms:
- Parametrized/empirical
- True quantum description

Dynamics:
- Classical Molecular dynamics
- Monte-Carlo
- Quantum dynamics

Interatomic interactions in atomistic modeling

$$V_{\mathrm{LJ}}(r) = \frac{A}{r^{12}} - \frac{B}{r^{6}},$$

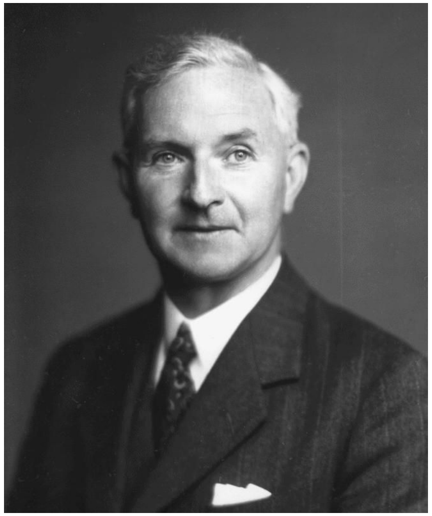


$$A = 4\varepsilon\sigma^{12} \quad B = 4\varepsilon\sigma^{6}$$

- in 1924 done for Ne and Ar gases
- in 1925 extended to Kr, Xe and like ions

For Kr using only:
1) interatomic distance and compressibility of RbBr
2) Refractivity of Br^{-}, Kr, Rb^{+}

Obtained for 32 ionic crystals:
1) Interatomic distance (2% accuracy for mono) predicted for MgSe (5%)
2) Compressibilities
3) Crystal energy



Sir John Edward Lennard-Jones

no electrons

1. Jones J. E. Proc. R. Soc. Lond. A106 (1924) 441–462; 463-477 (Articles by W.Bragg in the same vol)
2. Lennard-Jones J. E. Proc. R. Soc. Lond. A109 (1925) 584–597 (Articles by P.Dirac in the same vol)

Essential role of electrons in interatomic interaction

- 1897 discovery of electron by E.Wiechert and J. Thomson
- 1913 planetary model of atom by N. Bohr
- 1924 wave properties of electron suggested by Louis de Broglie and proved in 1927 in Davisson–Germer experiment
- 1926 Schrödinger equation - for wave functions and can describe electrons correctly

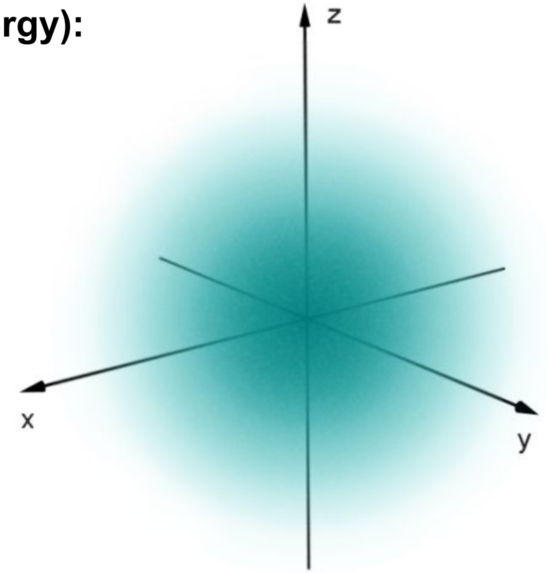
Time dependent SE (*ψ* - wave function, *H* - operator of total energy):

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \hat{H}\psi(\mathbf{r},t)$$

$$\hat{H}\Psi(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_N) = E\Psi(\vec{r}_1,\vec{r}_2,\cdots\vec{r}_N)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)$$

kinetic energy + potential energy



Orbital s ($\ell = 0$, $m_\ell = 0$)

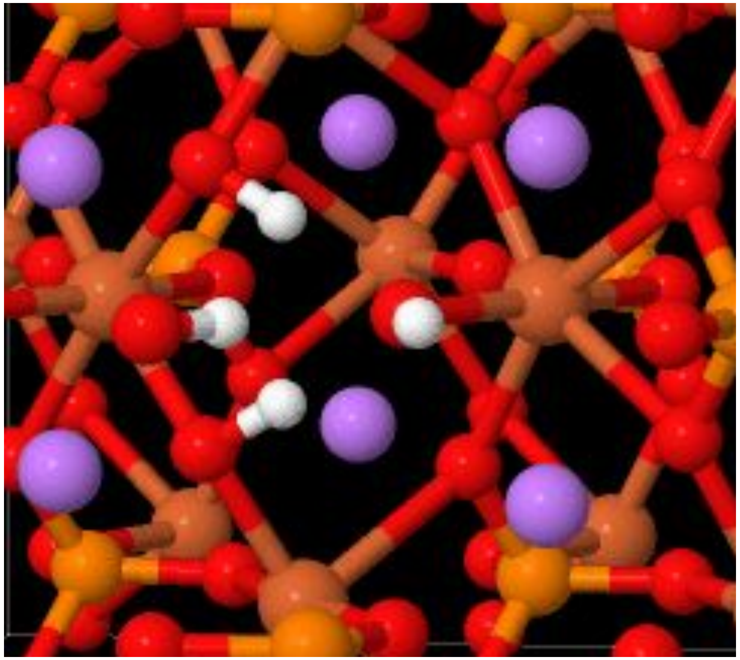
E=-13.6 eV

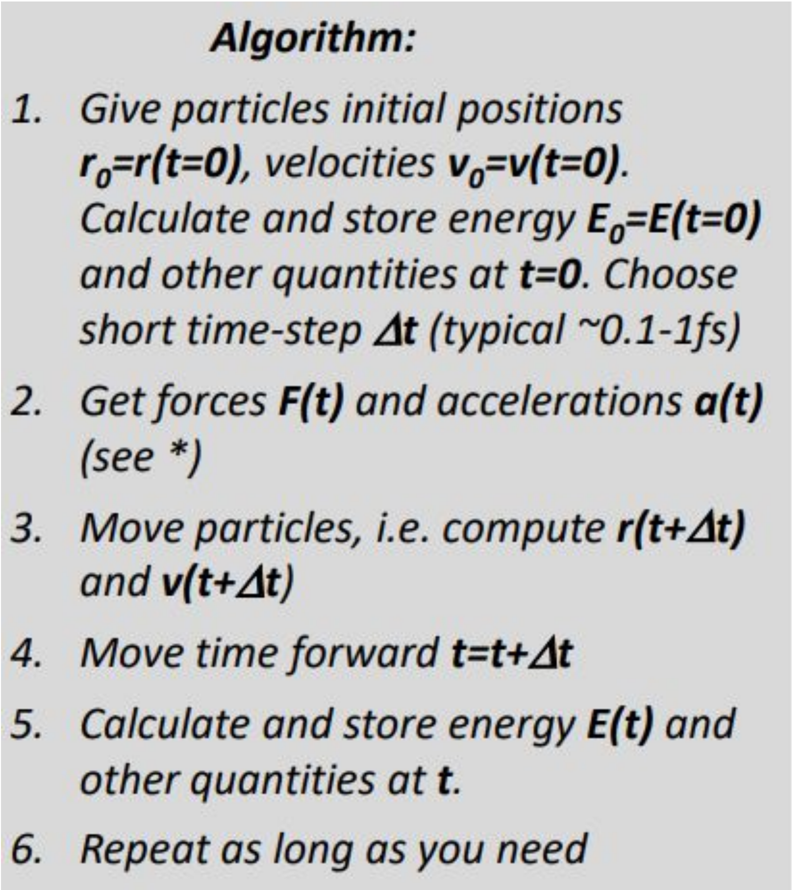
Molecular dynamics method

- Solve Newtonian equation of motion for N classical particles (3N coupled equations)
- The force between atoms is determined either from DFT or using classical force field

$$\mathbf{F} = m\mathbf{a}$$

$$E_{\mathrm{tot}} = \sum_{i=1}^{N} \tfrac{1}{2} m_i \mathbf{v}_i^2 + V(\mathbf{r}) \qquad -\frac{dV}{d\mathbf{r}} = m\frac{d^2\mathbf{r}}{dt^2}$$





Algorithm:

1. *Give particles initial positions* ***r**$_0$**=r(t=0)**, velocities **v**$_0$**=v(t=0)**. Calculate and store energy **E**$_0$**=E(t=0)** and other quantities at **t=0**. Choose short time-step **Δt** (typical ~0.1-1fs)*
2. *Get forces **F(t)** and accelerations **a(t)** (see *)*
3. *Move particles, i.e. compute **r(t+Δt)** and **v(t+Δt)***
4. *Move time forward **t=t+Δt***
5. *Calculate and store energy **E(t)** and other quantities at **t**.*
6. *Repeat as long as you need*

Aksyonov et al. Inorg. Chem. 2021, 60, 5497−5506

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- Basics of quantum level atomistic modeling (DFT)

Scheme of co-precipitation synthesis

1. Prepare solutions ✓
- Dissolve Ni, Mn, Co nitrates in water
- Prepare prec and complex agents
- pH adjustments

2. Co-precipitation ✓
- Add precipitation agent into nitrates
- Stir

3. Filter
- Filter and wash

4. Drying
- Dry at 100 - 150 C

5. Mix with Li
- Produce fine powder
- mix with Li_2CO_3

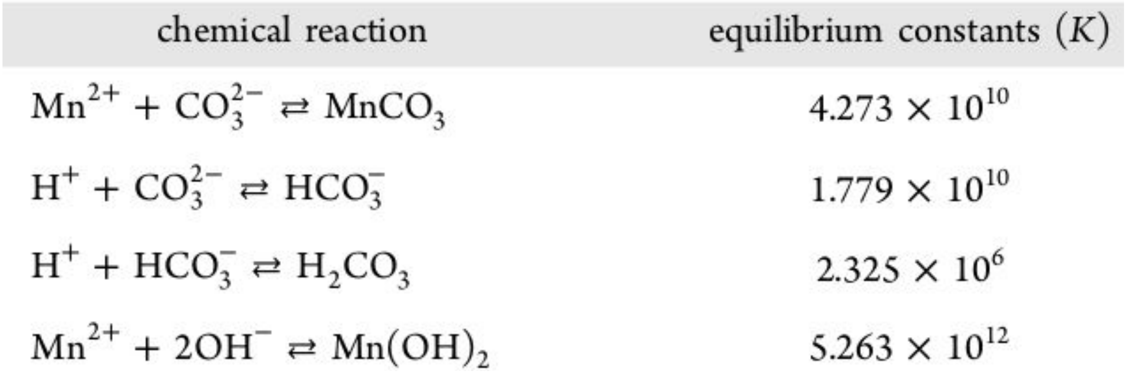
6. Sinter ✓
- Sinter at 700-900 C

Step 1. Prepare solutions, e.g. $MnSO_4$ + NH_4HCO_3

- pH level is important for precipitation
- To calculate equilibrium concentrations of species the following system of nonlinear equations should be solved:

$$\begin{aligned}\bar{c}_{\mathrm{Mn}^{2+}} = {} & [\mathrm{Mn}^{2+}] + [\mathrm{MnCO_3}] + [\mathrm{Mn(OH)_2}] \\ & + [\mathrm{Mn(NH_3)}]^{2+} + [\mathrm{Mn(NH_3)_2}]^{2+} \\ & + [\mathrm{Mn(NH_3)_3}]^{2+} + [\mathrm{Mn(NH_3)_4}]^{2+} \end{aligned} \qquad (1)$$

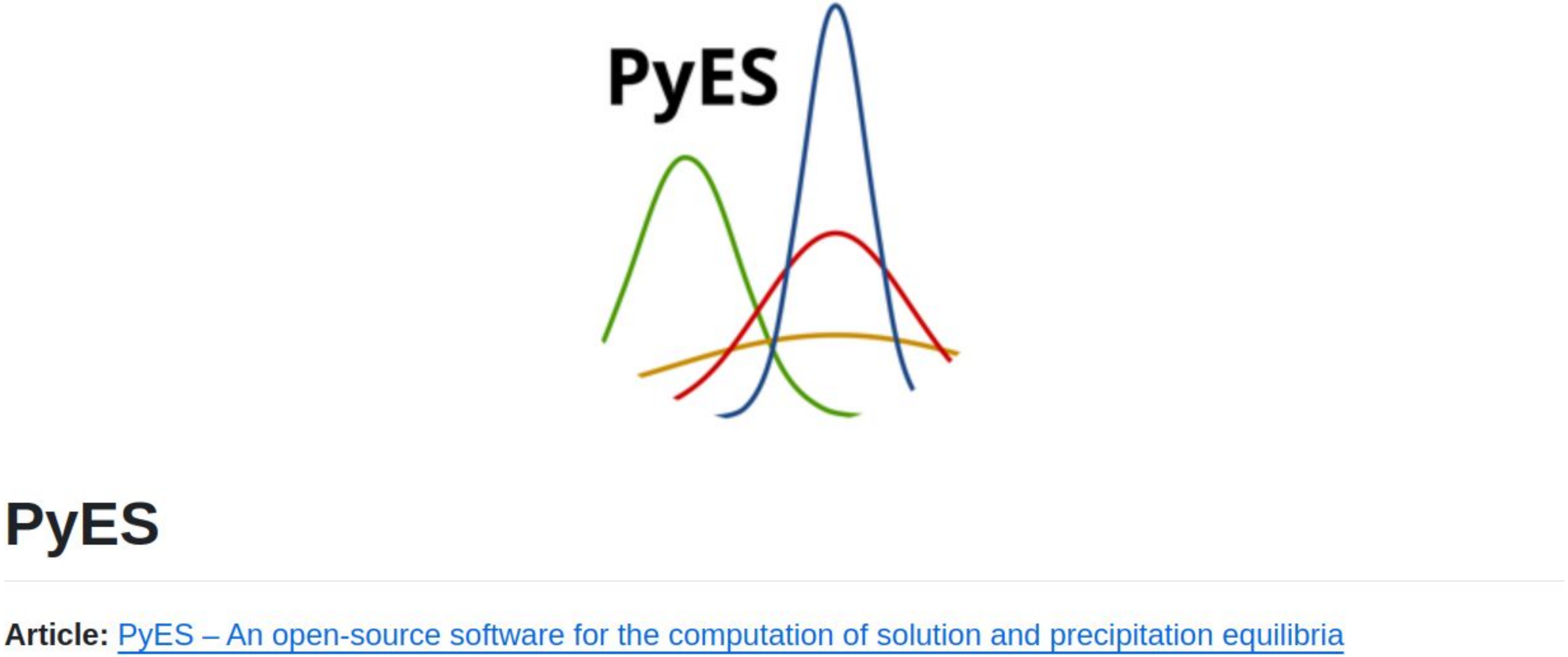
$$\bar{c}_{\mathrm{HCO_3^-}} = [\mathrm{HCO_3^-}] + [\mathrm{H_2CO_3}] + [\mathrm{CO_3^{2-}}] + [\mathrm{MnCO_3}] \qquad (2)$$



chemical reaction	equilibrium constants (K)
$Mn^{2+} + CO_3^{2-} \rightleftarrows MnCO_3$	4.273×10^{10}
$H^+ + CO_3^{2-} \rightleftarrows HCO_3^-$	1.779×10^{10}
$H^+ + HCO_3^- \rightleftarrows H_2CO_3$	2.325×10^{6}
$Mn^{2+} + 2OH^- \rightleftarrows Mn(OH)_2$	5.263×10^{12}

Python library to compute concentrations

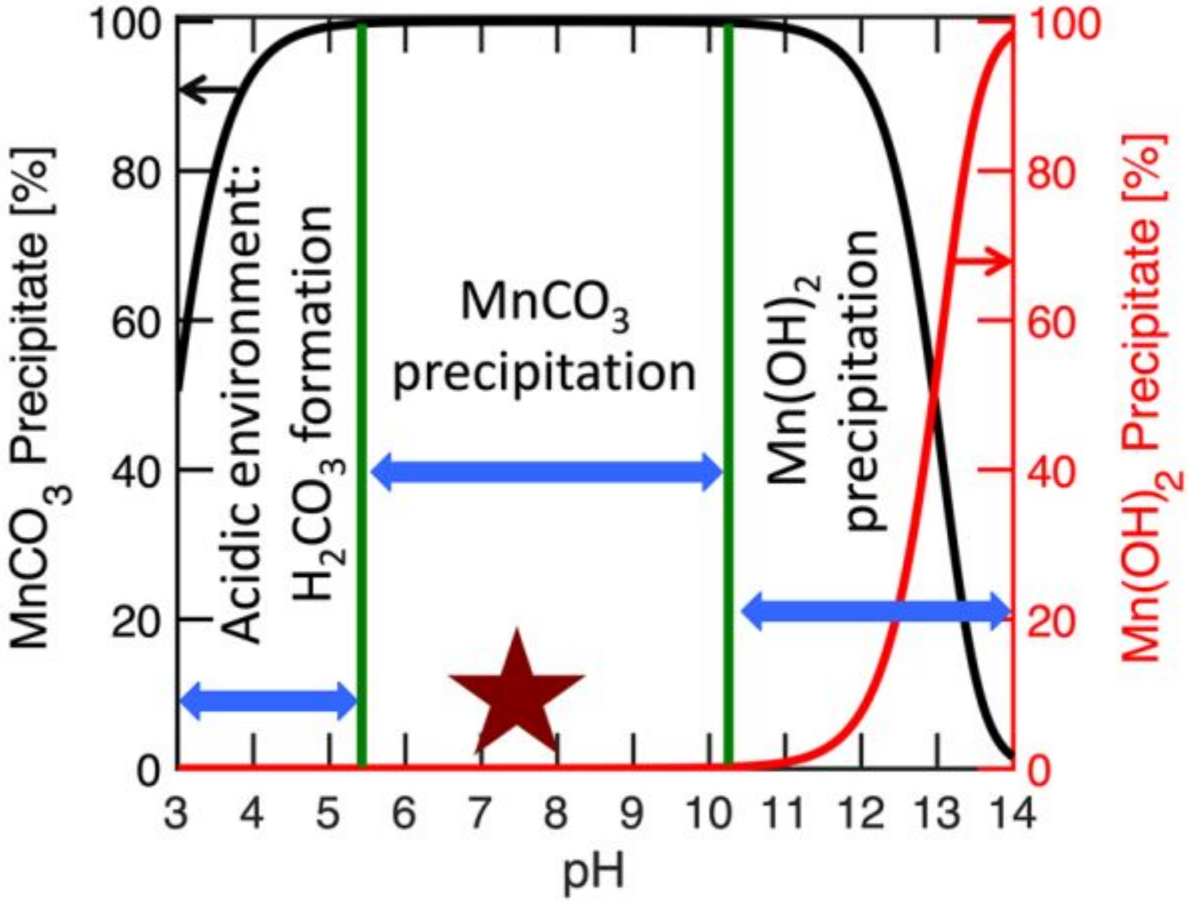
https://github.com/Kastakin/PyES



PyES

Article: PyES – An open-source software for the computation of solution and precipitation equilibria

Solution pH dependent precipitation of $MnCO_3$



Let's choose pH=7.5

Step 2. Modeling of co-precipitation

Co-precipitation should be achieved (depends on solubility, pH, surface, mixing)

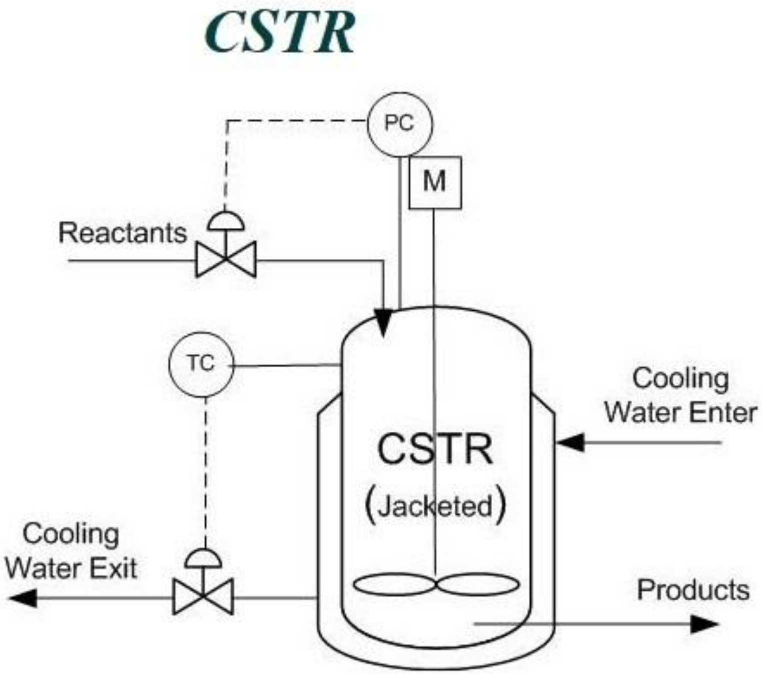
1. Ion behaviour is solution (role of complexing agents) MD
2. pH-dependence, how to avoid selective precipitation, calculate solubility limits MD
3. Surface chemistry of particles (Ni, Mn, Co distribution on surface, adsorption of ligands -> particle morphology)
4. Homogeneity (segregation, phase separation)
5. Morphology and particle size control
   a. computational fluid dynamics (CFD) - mixing and stirring conditions

Predictions:

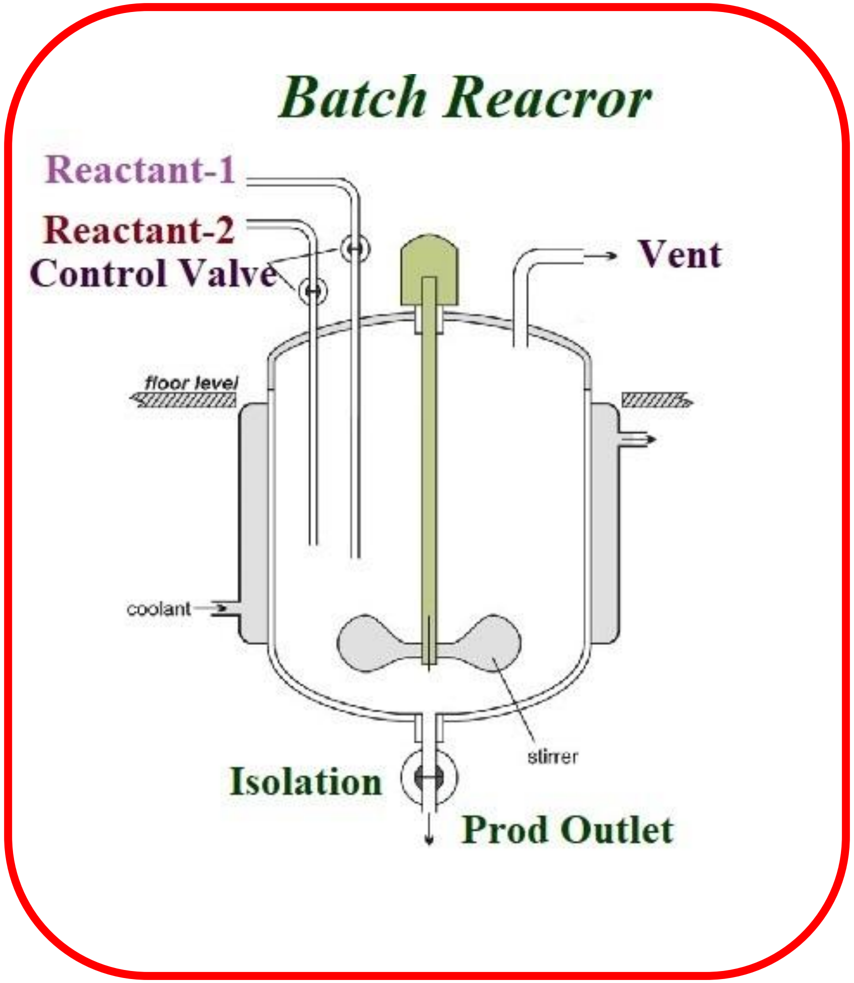
1. Optimize pH, temperature, concentrations, stirring
2. Defects during co-precipitation

Step 2. Co-precipitation:

Types of co-precipitation reactors: проточный + стационарный

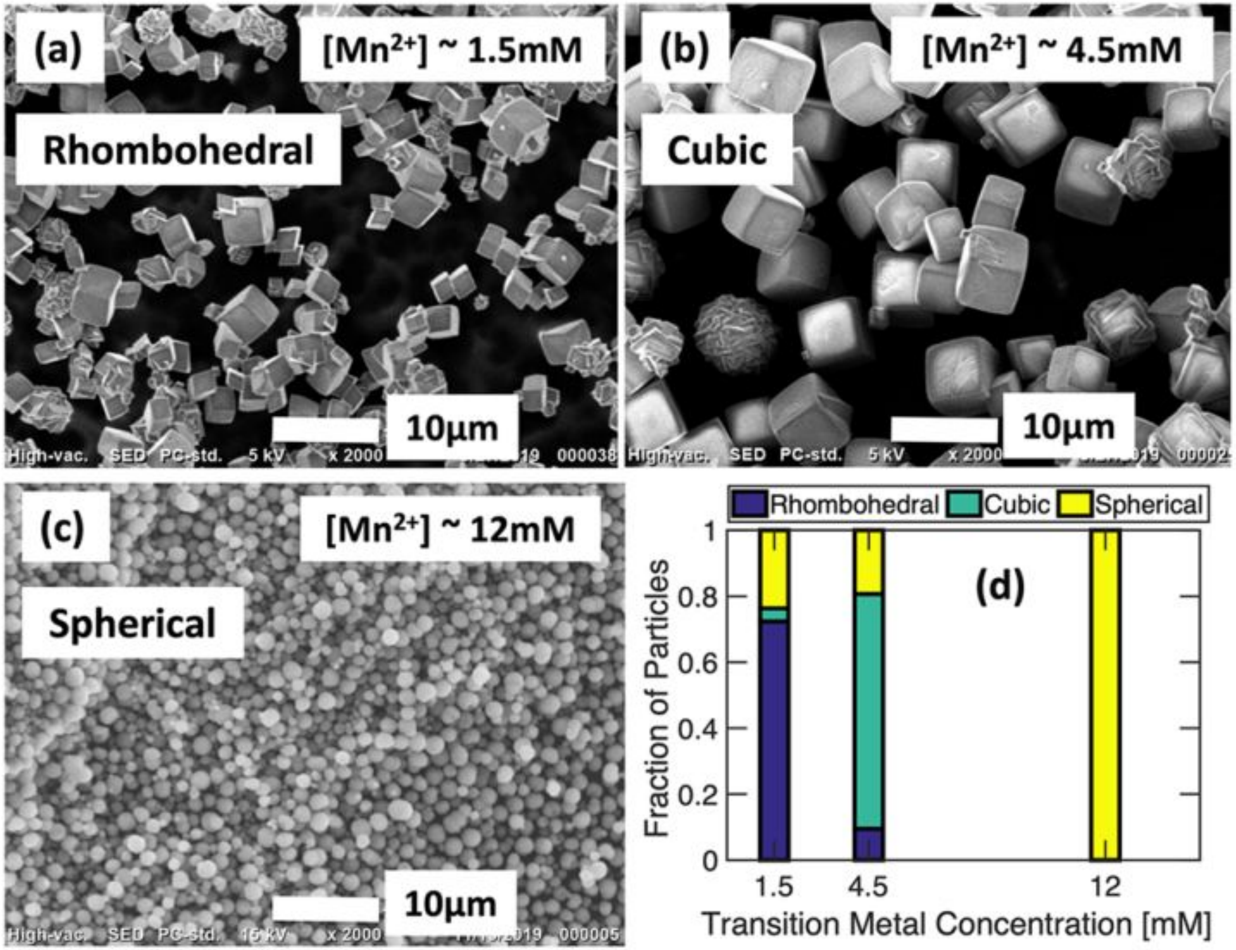


A continuous stirred tank reactor



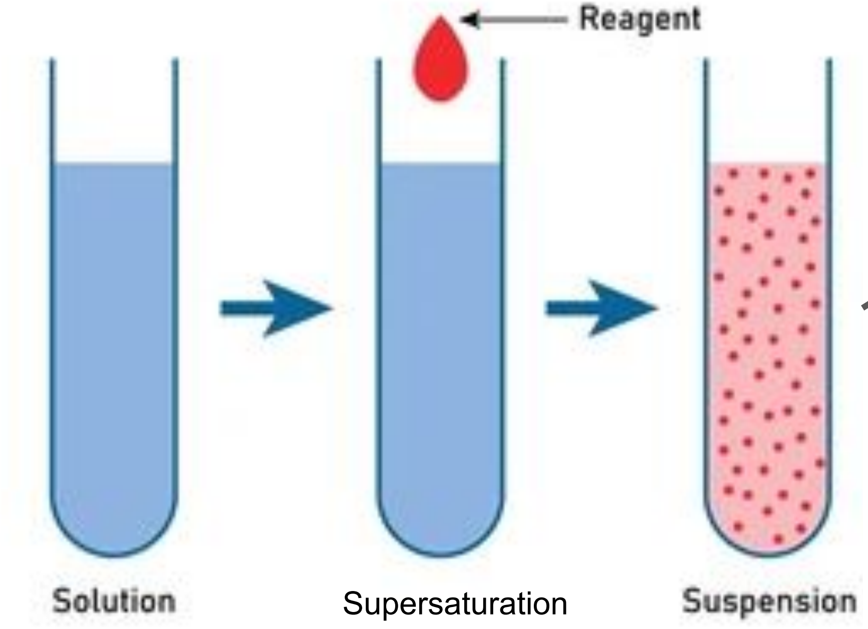
Step 2. Co-precipitation. Impact of Mn^{2+} concentration

Batch reactor precipitation

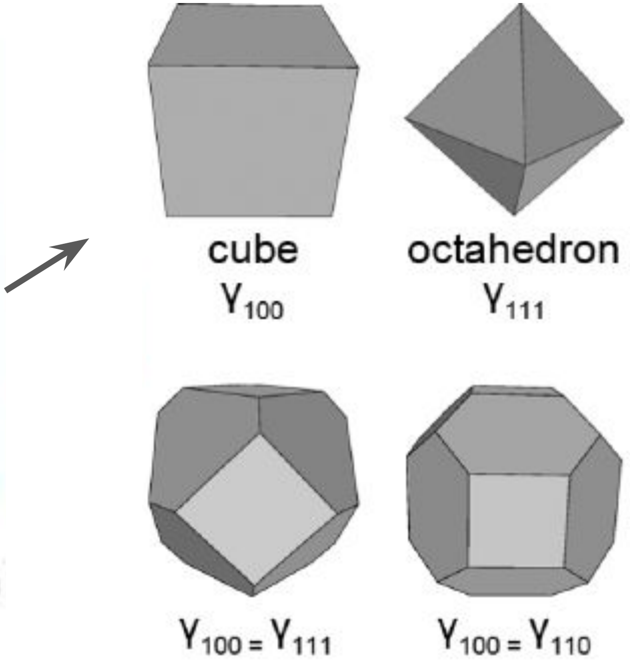


?

What governs particle morphology?
Thermodynamics vs kinetics?

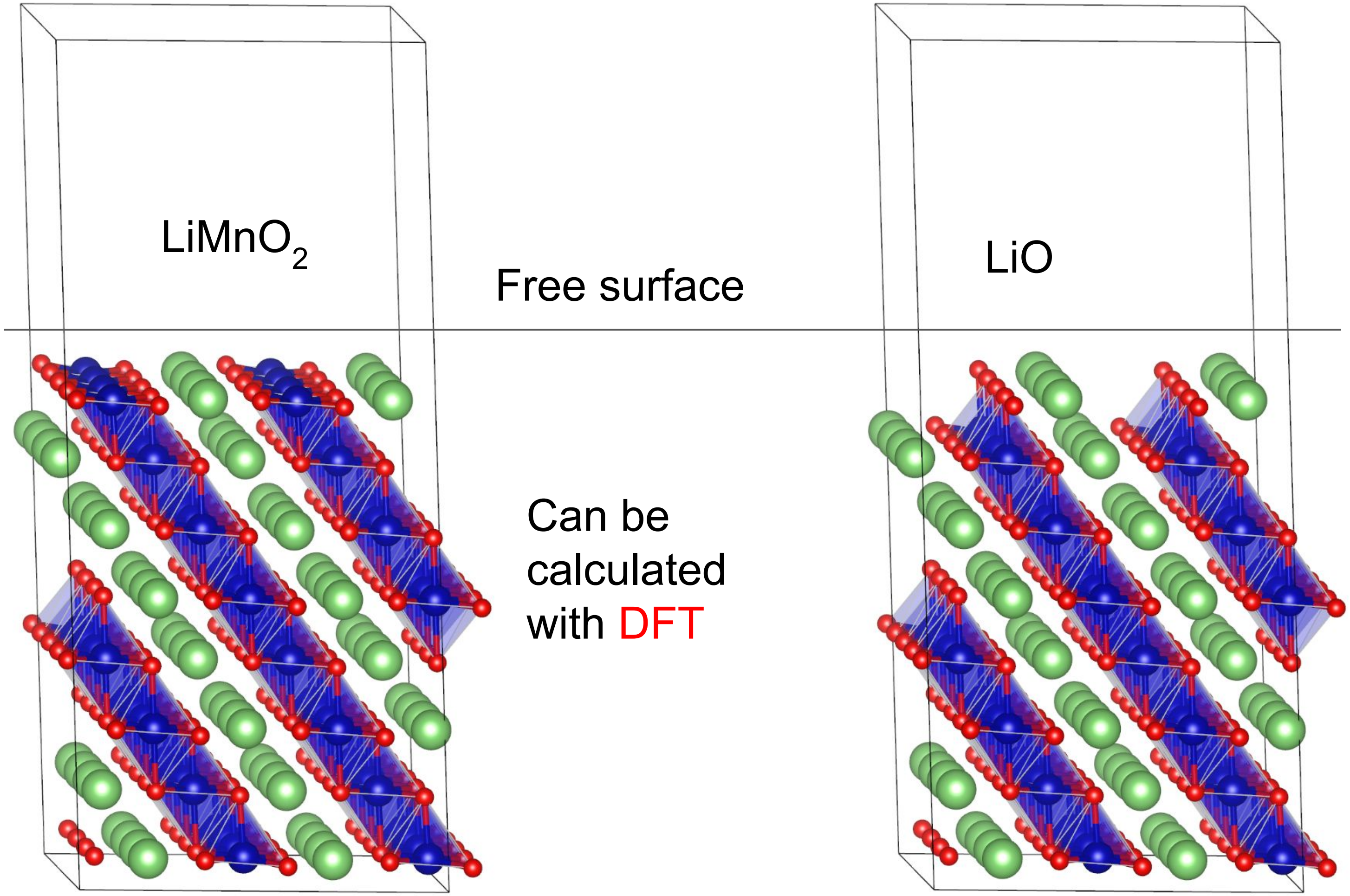


Precipitation process



Assuming that only **thermodynamics** matters, the shape of particle is defined by its **surface energy**

Surface energy γ (J/m^2), role of stoichiometry

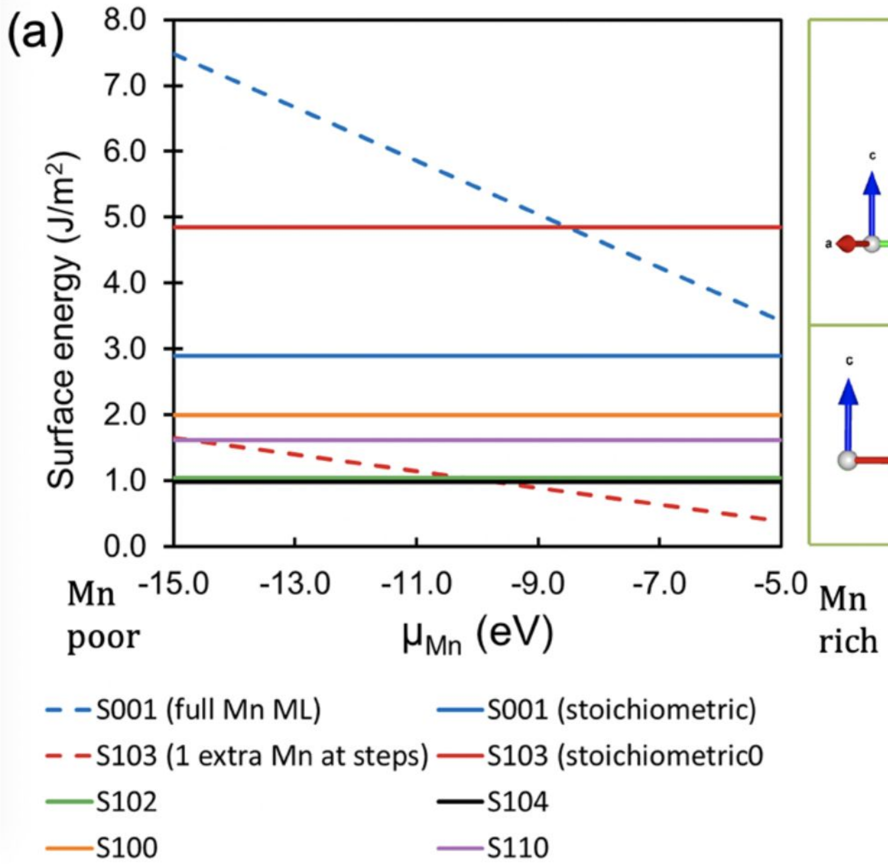


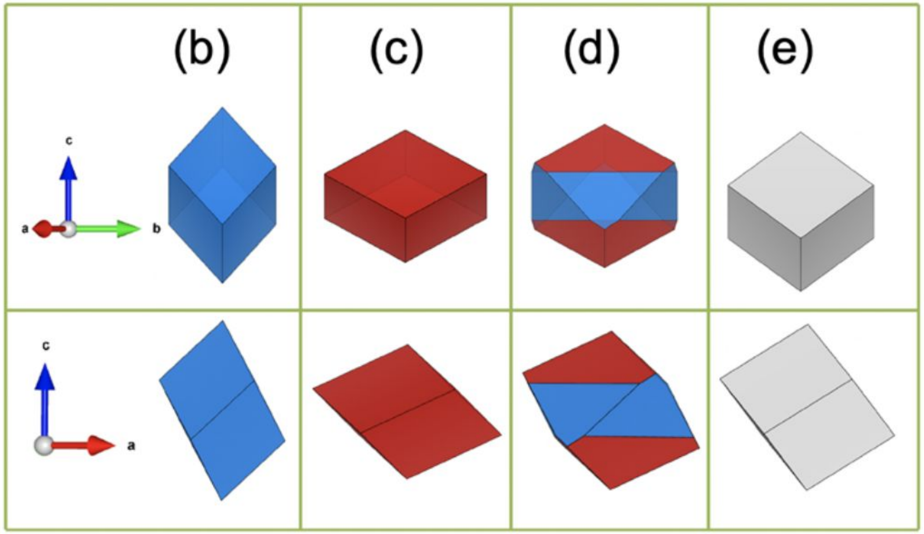
Can be calculated with DFT

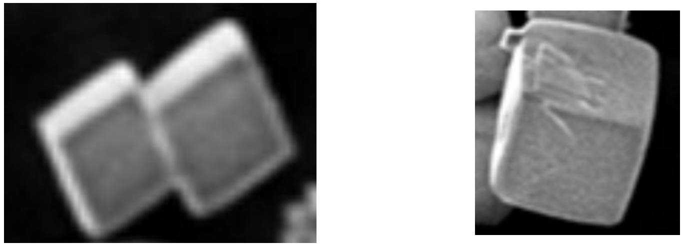
$$\gamma = \frac{1}{2A}\left(E_{\mathrm{slab}} - E_{\mathrm{bulk}}\right)$$

$$\gamma = \frac{1}{2A}\left(E_{\mathrm{slab}} - E_{\mathrm{bulk}} + \sum_i \Delta_i \mu_i\right)$$

Surface energy as a function of Mn^{2+} chemical potential





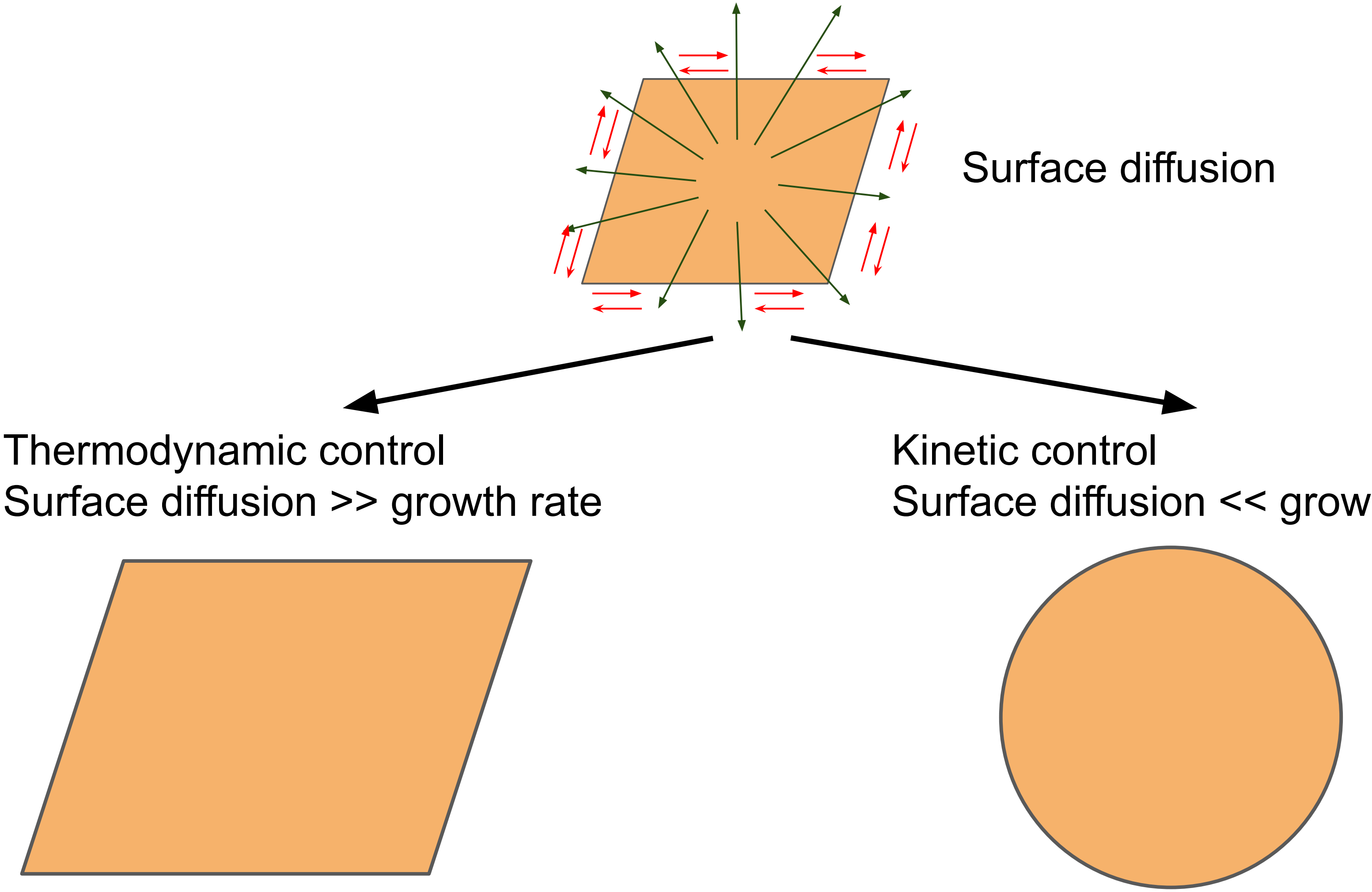


$$\mu_i = \mu_i^\circ + RT \ln a_i,$$

Chemical potential of Mn^{2+} can be taken from experimental tables, or **calculated with Molecular dynamics** of solvation

How do spherical particles appear?

We assumed that the shape of particle is governed with thermodynamics, but what about kinetics?



Particle growth directions

Surface diffusion

Thermodynamic control
Surface diffusion >> growth rate

Kinetic control
Surface diffusion << growth rate

Modeling of particles growth with mesoscale model

Atomistic modeling is challenging, the particle growth rate is 10 μm/min
1 μm particle of $MnCO_3$ has 4.28×10^{10} (43 billion) atoms,
Therefore mesoscale phase-field methods are used

- ξ is phase variable 1 for liquid phase, -1 for precipitate, 0 for interface
- ξ changes smoothly eliminating necessity to track sharp interfaces
- Concentration c_{Mn2+} and c_{CO32-} varies within the liquid phase.
- Driving forms for precipitation *s* comes from supersaturation $c1*c2/K_{SP}$

$$\tau\frac{\partial\xi}{\partial t} = -\frac{\delta F}{\delta\xi} = -\left(\frac{\partial F}{\partial\xi} - \vec{\nabla}\cdot\frac{\partial F}{\partial\vec{\nabla}\xi}\right)$$

F is energy functional
τ is time constant of reaction rate

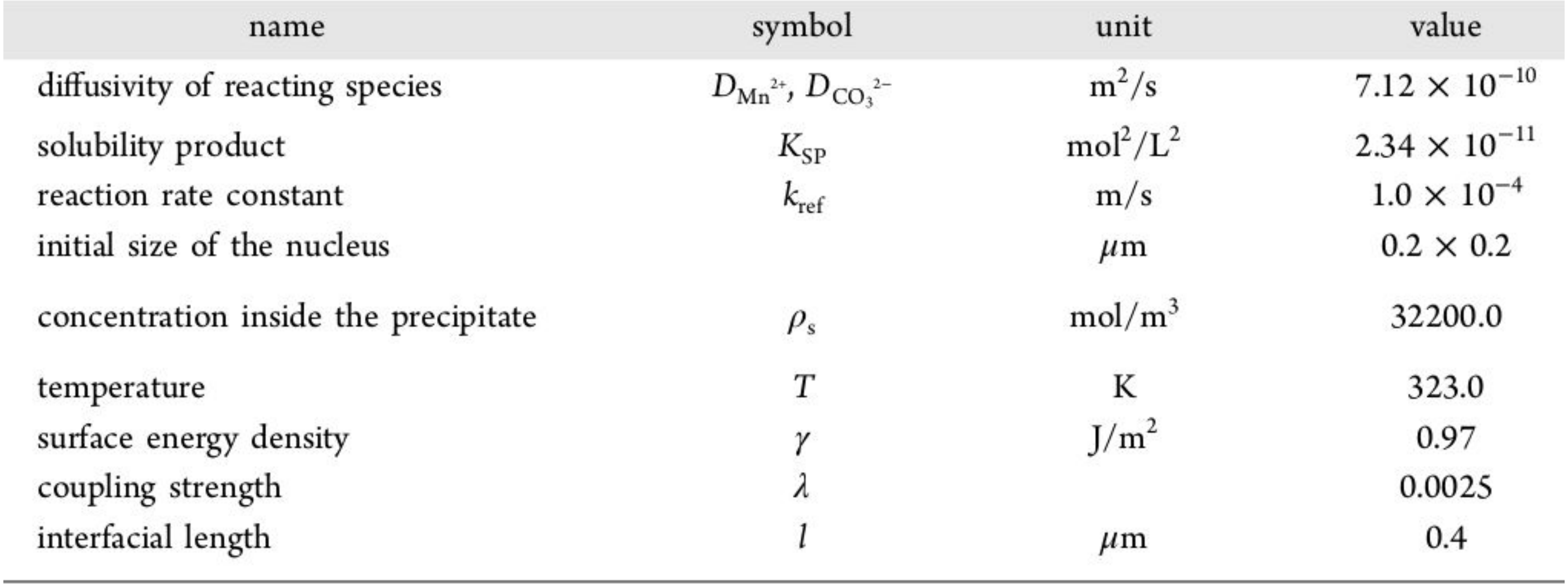
$$F(\xi, c) = \int\Big(\underbrace{((1/2)\cdot((\epsilon A(\hat{n}))^2\cdot|\vec{\nabla}\xi|^2))}_{\text{Surface energy}} + \underbrace{f(\xi, c)}_{\text{Supersaturation}}\Big)\,dV$$

Diffusion

$$\frac{\partial c_i}{\partial t} = \vec{\nabla}\cdot(D_i\vec{\nabla}c_i) + A_1\frac{\partial\xi}{\partial t}$$

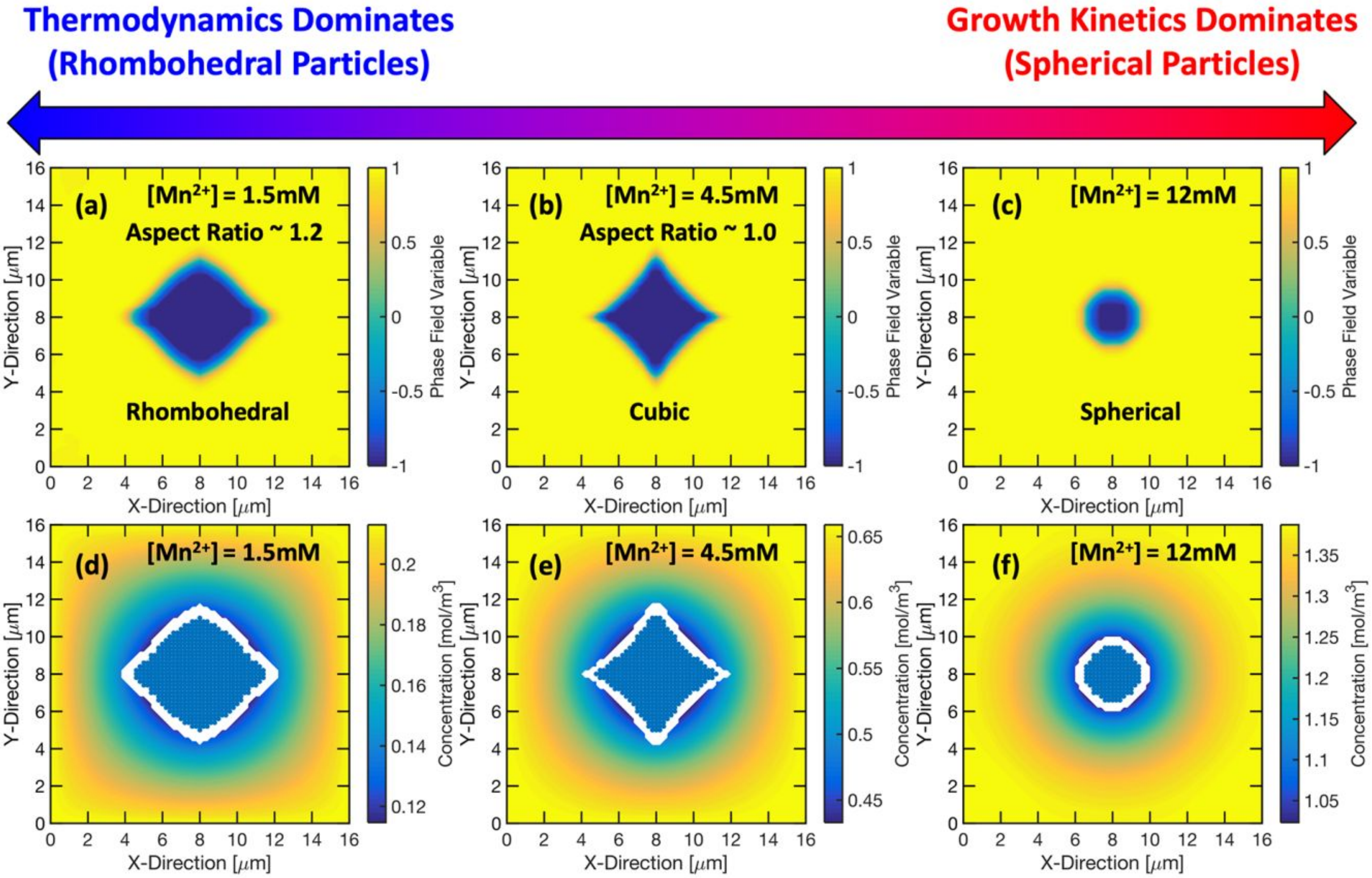
c is concentration
A_1 related to SP

Parameters of the phase field model



name	symbol	unit	value
diffusivity of reacting species	$D_{\mathrm{Mn}^{2+}}$, $D_{\mathrm{CO}_3^{2-}}$	m^2/s	7.12×10^{-10}
solubility product	K_{SP}	mol^2/L^2	2.34×10^{-11}
reaction rate constant	k_{ref}	m/s	1.0×10^{-4}
initial size of the nucleus		μm	0.2×0.2
concentration inside the precipitate	ρ_s	mol/m^3	32200.0
temperature	T	K	323.0
surface energy density	γ	J/m^2	0.97
coupling strength	λ		0.0025
interfacial length	l	μm	0.4

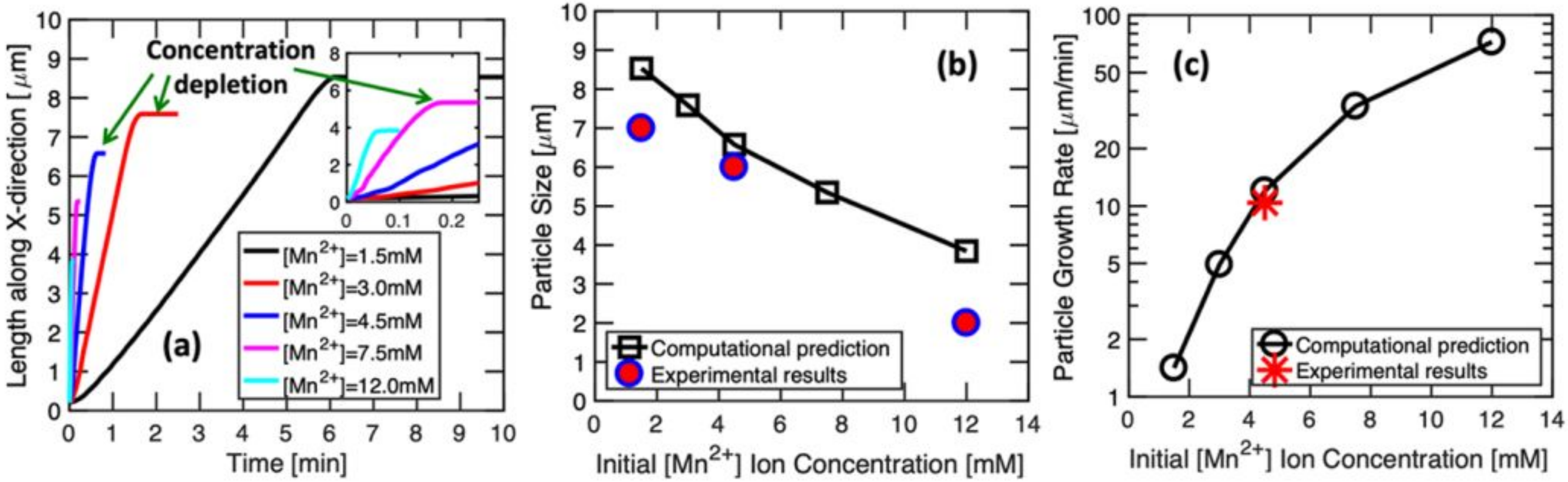
Results of phase field modeling



Thermodynamics Dominates
(Rhombohedral Particles)

Growth Kinetics Dominates
(Spherical Particles)

Particle growth rate

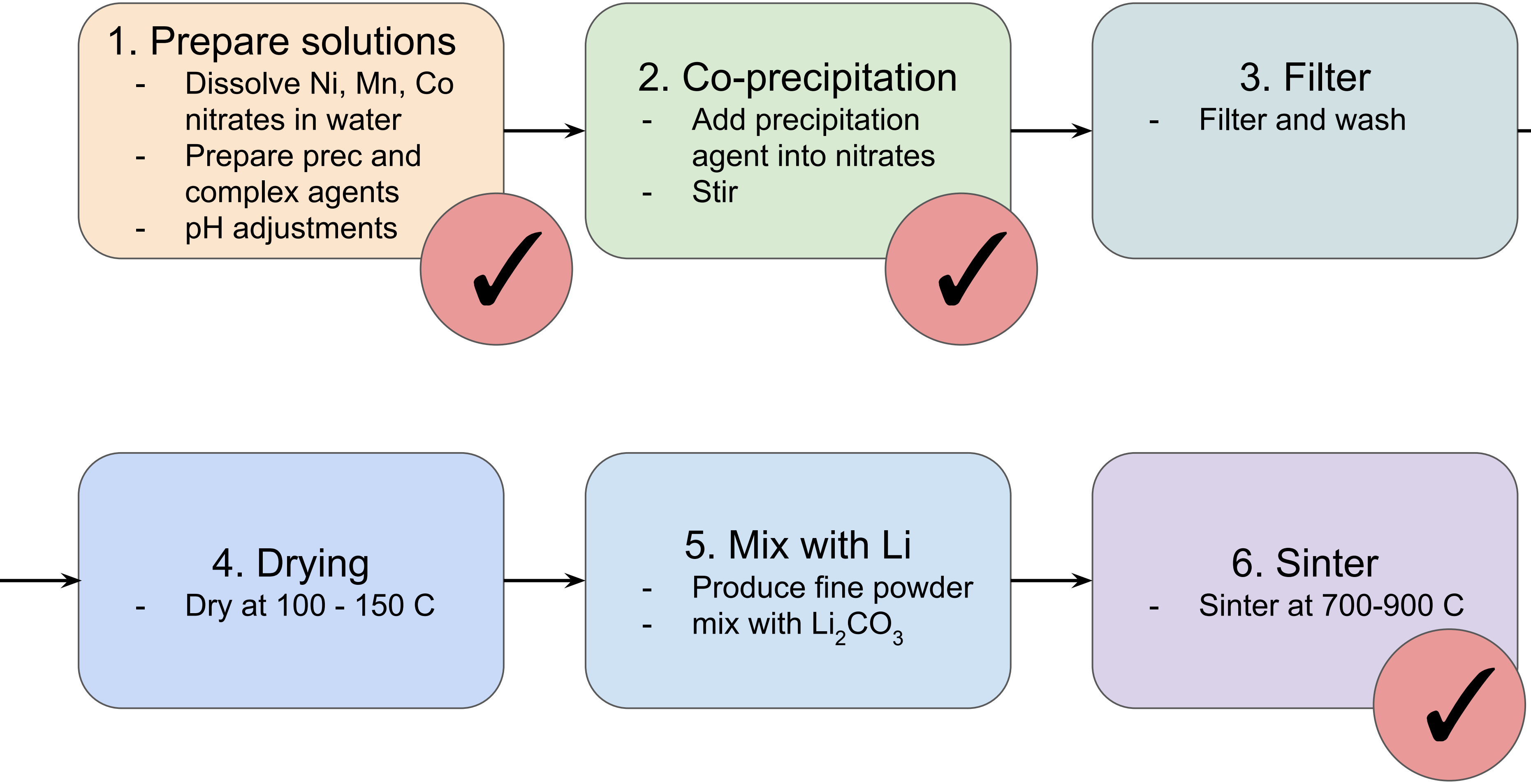


Summary

The growth of precipitates is controlled by energy of free surface, surface diffusion and growth rate

- Small concentration of ions -> small oversaturation -> slow growth -> the shape is controlled thermodynamically
- Large concentration of ions -> strong oversaturation -> high growth -> the shape is controlled kinetically - spherical
- Surface energies is calculated with **DFT**
- Chemical potential and diffusivity is taken from experiment, but can be also calculated using **molecular dynamics**.
- The growth of precipitates is modelled with phase-field model based on parameters calculated with DFT and taken from experiment

Scheme of co-precipitation synthesis



1. Prepare solutions ✓
   - Dissolve Ni, Mn, Co nitrates in water
   - Prepare prec and complex agents
   - pH adjustments
2. Co-precipitation ✓
   - Add precipitation agent into nitrates
   - Stir
3. Filter
   - Filter and wash
4. Drying
   - Dry at 100 - 150 C
5. Mix with Li
   - Produce fine powder
   - mix with Li_2CO_3
6. Sinter ✓
   - Sinter at 700-900 C

Step 6. Solid State Synthesis (**sintering**)

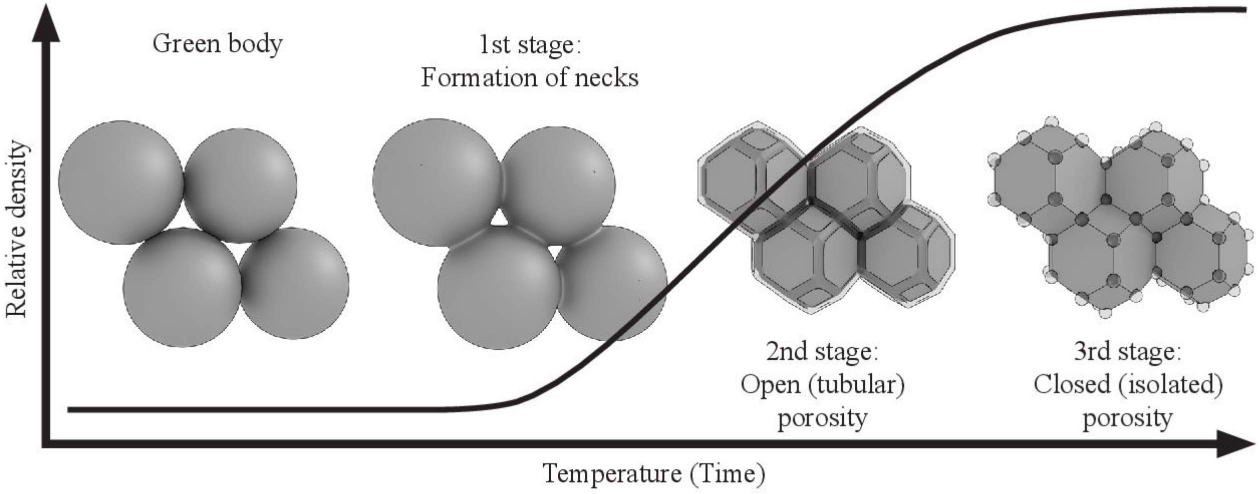


Figure 6: Stages of sintering.

For NMC: $MnCO_3 + Li_2CO_3$ -> $LiMnO_2 + 2CO_2$

Remove CO_3 and introduce Li.

Processes:

- Densification, removal of pores
- Reaction between two phases with the formation of a new phase
- Diffusion of transition elements
- CO_2 removal

Step 6. Solid State Synthesis (**sintering**)

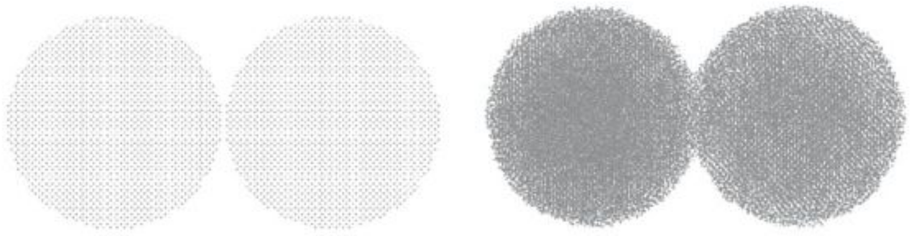
Why modeling can be useful?

- Predict how particle size, sintering time, T influence grain growth,
- Sintering atmosphere and partial pressure affect phase stability, oxidation states, defects
- What is the final size distribution and morphology

What tools can be used?

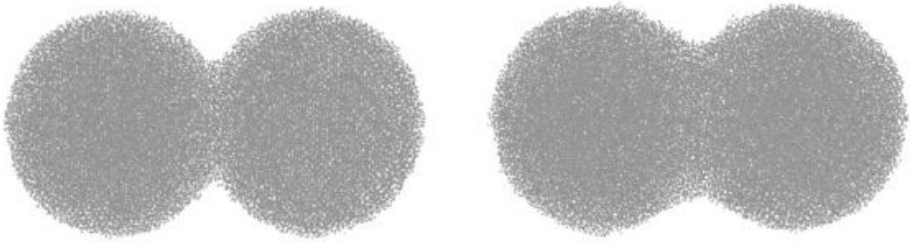
- DFT, Thermodynamics, Molecular Dynamics, Monte-Carlo, Phase-Field Modeling, Finite Elements;
- The complete description is challenging, but individual processes can be addressed:
    - impact of Li-excess and O_2 partial pressure on particle morphology
    - diffusion of transition metals and other elements to estimate required sintering times
    - segregation of dopants

MD EAM simulation of W particles sintering



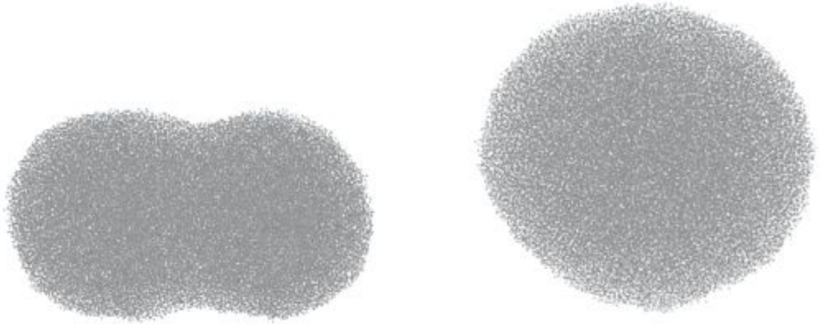
(a) 500 K (initial temperature), 0s

(b) 1000K, 10 ps



(c) 1500 K, 20 ps

(d) 2000 K, 30 ps



(e) 2500 K, 40 ps

(f) 3000 K, 50 ps

Fig. 5. Sintering response of W nanoparticle based on atomistic simulation.

- Small-sized powder enables sintering at lower temperatures
- Revealed pre-melting on surface layer that gives low activation energy

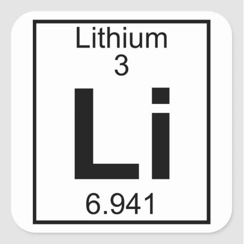
A. Moitra et al. / Acta Materialia 58 (2010) 3939–3951

Plan of lecture

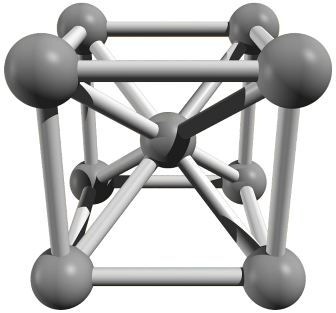
- Short introduction to materials modeling
- How to model/approach co-precipitation synthesis of cathode material?
- Basics of quantum level atomistic modeling (DFT)

First principles or *ab initio* approach

Quantum chemistry allowed description of matter from first principles without any information from experiment, except for fundamental constants, such as electron mass, charge and planck constant



$$\longrightarrow \quad \hat{H}\psi = E\psi \quad \longrightarrow$$



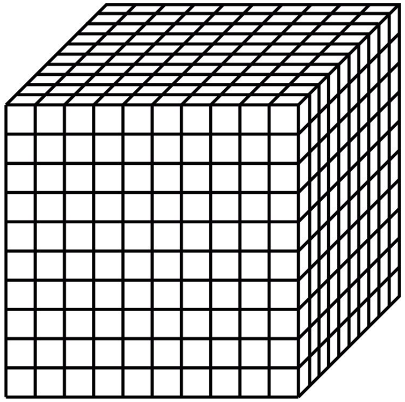
INPUT:
- Atomic number - 3
- Number of atoms in unit cell - 1

OUTPUT:
- Metall, $E_{cohesive}$ = 1.63 eV/atom
- bcc lattice with a = 3.51 A at room T
- Electronic structure and possibility to derive all properties corresponding to ideal crystal

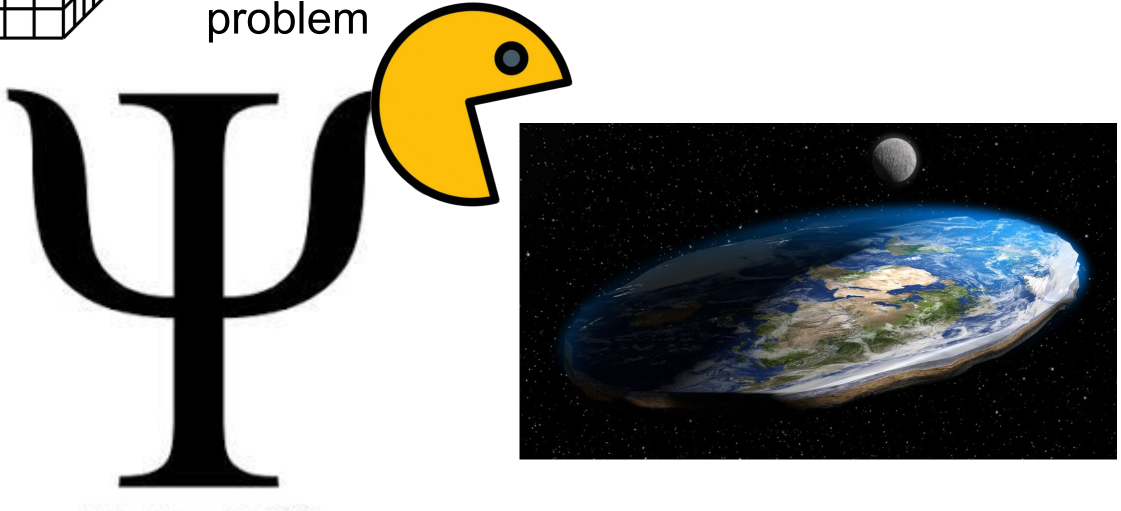
In principle the calculated properties will match experiment almost exactly!
I.e. quantum mechanics completely describes chemical interactions, **but ....**

Quantum description is very complex to treat!

Ψ(r1, r2, .. rn, R1, R2, RN) is a complex function depending on 3n +3N coordinates.
The analytical solution is available only for H_2 therefore numerical methods are used.
To write down Ψ numerically with only 10 values for each coordinate (just the real part without spin):



1 electron - 10^3 ~ 1 KB
2 electrons - 10^6 ~ 1 MB
5 electrons - 10^{15} ~ 1000 TB
8 electrons - 10^{24} ~ **1000 ZB**, Zettabyte
The total storage capacity of all computers on Earth is **60 ZB**
The solution complexity is faster than exponential with respect to number of electrons due to combinatorial nature of the problem



We need approximations! There are four of them.

Approximation 1: Born-Oppenheimer

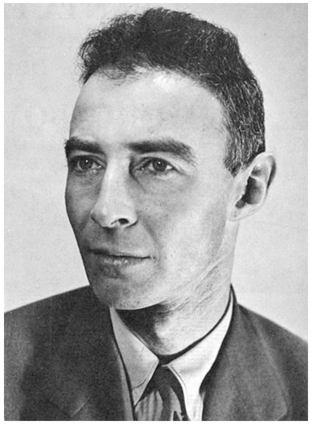
Since nuclei are much heavier than electrons (m_p = 1835 m_e), their dynamics can be decoupled and considered separately:

a. Froze cores -> solve electrons -> solve cores classically (error scales as $(M/m_e)^{-1/4}$)

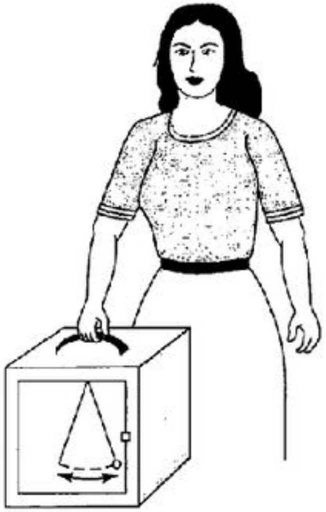
b. Reduces number of variables and simplifies the problem

c. Oftenly used in calculations introducing only small error for ground state

Max Born

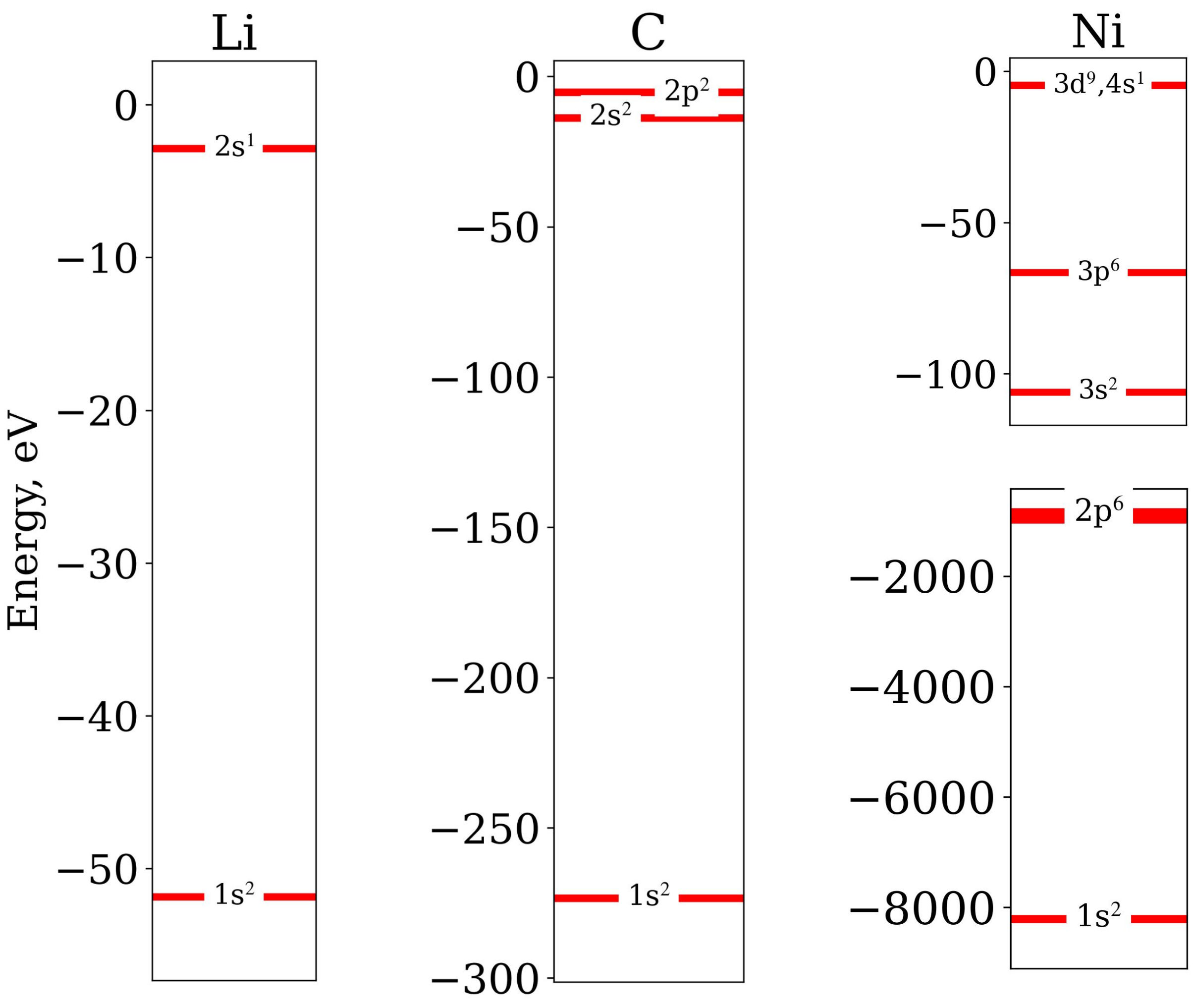


Robert Oppenheimer

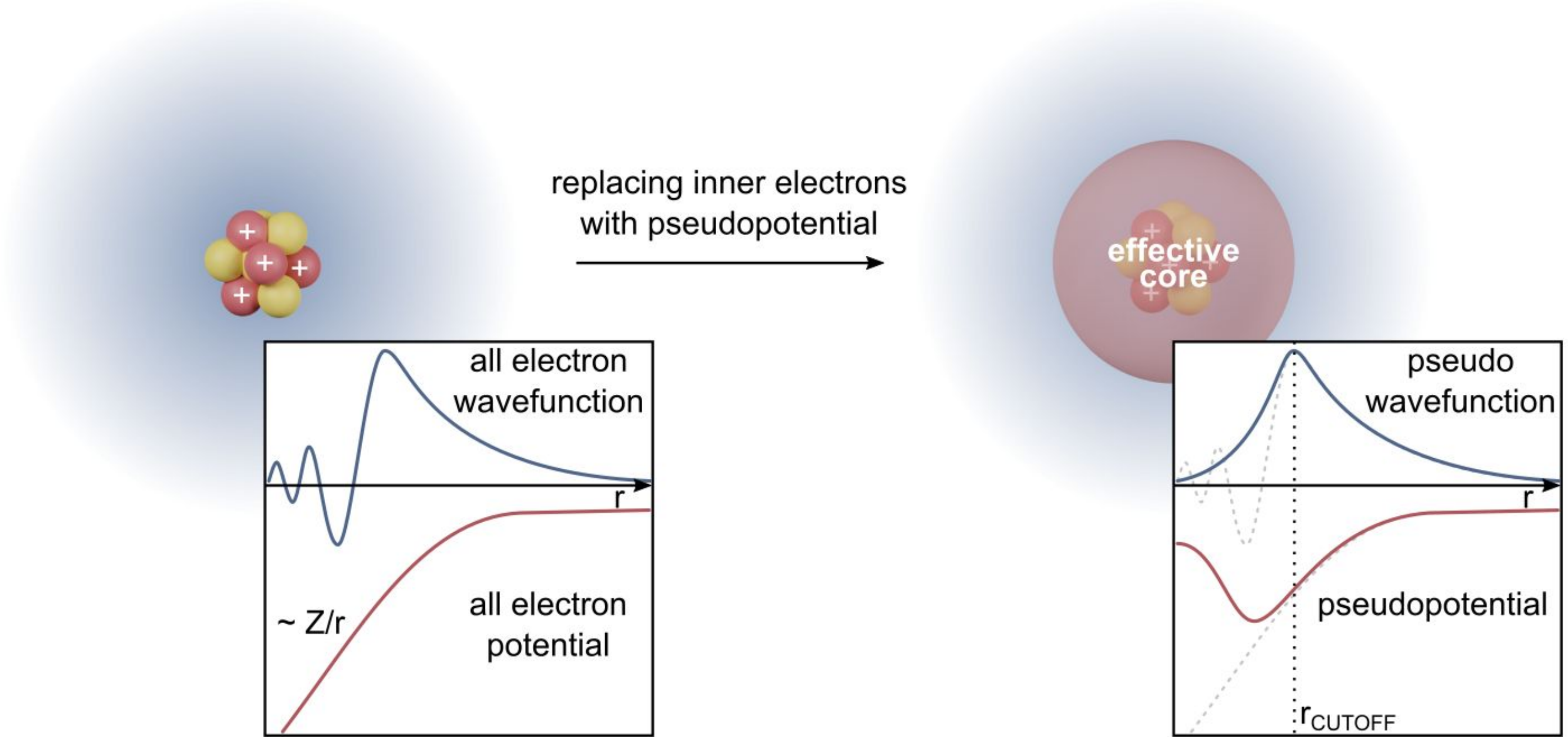


Approximation 2: deals with core electrons

Valence shell: $2s^1$ $2s^22p^2$ $3d^94s^1$ (only 10 out of 28!)



Approximation 2: Replace core electrons with pseudopotential

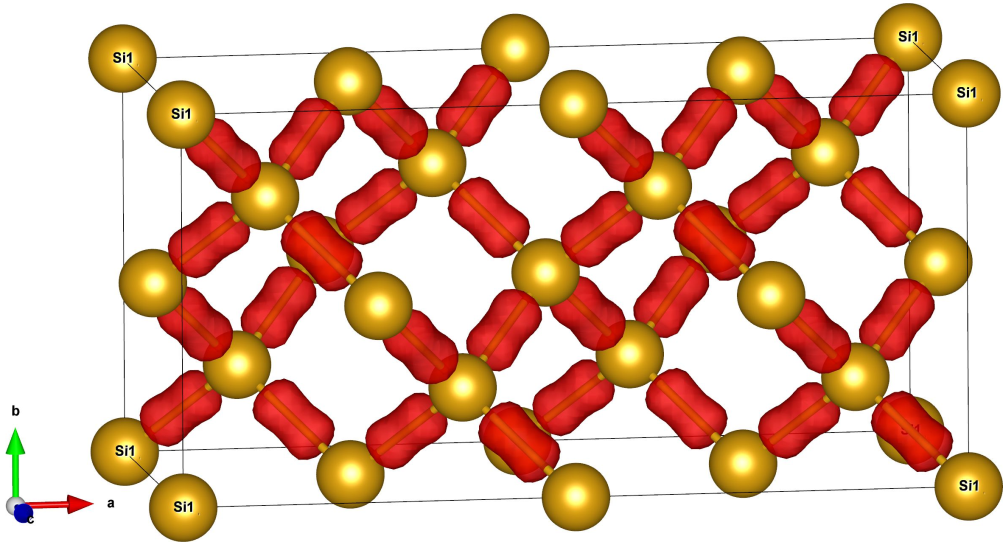


PAW - *projected augmented wave*, introduces only small error compared to full electron description

Approximation 3: electronic density (actually not)

Use electronic density: $\mathbf{\Psi(r_1, r_2, \ldots, r_N)} \longrightarrow \mathbf{n(x, y, z)}$

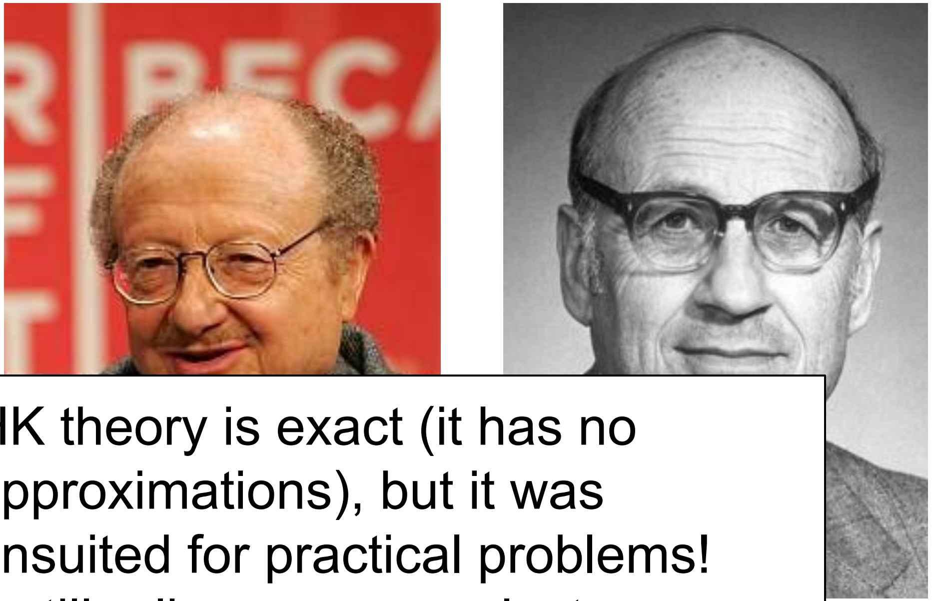
$$n(\mathbf{r}) = N \int \mathrm{d}^3\mathbf{r}_2 \cdots \int \mathrm{d}^3\mathbf{r}_N \, \Psi^*(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$



Electronic density is observable

Hohenberg-Kohn proved that 3 is not an approximation

- The idea of using electron density for calculations of solid was first used in semi-classical orbital-free Thomas-Fermi theory (1927); but the accuracy was quite low due to kinetic energy approximation.
- In 1964 Hohenberg and Kohn proved two important theorems according to which the electronic density is equivalent to many body wave functions in the sense that the total energy and all other properties are uniquely determined by density.



HK theory is exact (it has no approximations), but it was unsuited for practical problems!
It still relies on many-electron wave function to get density

998

1st theorem:

$$E = F[n(\mathbf{r})] + \int V_{ext}(r) n(\mathbf{r}) d\mathbf{r}$$

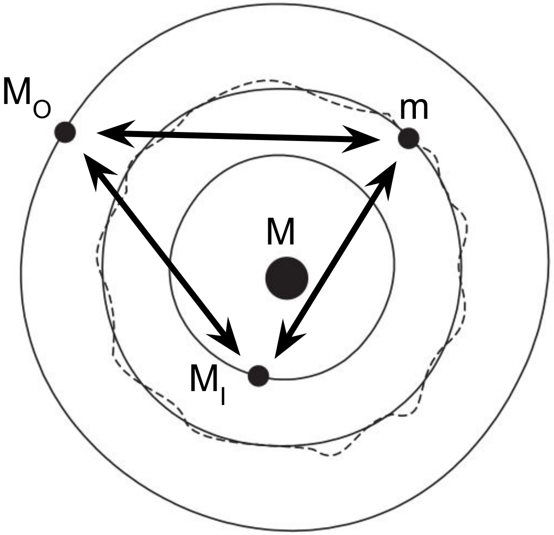
V_{ext} is potential created by nuclei

2nd theorem:

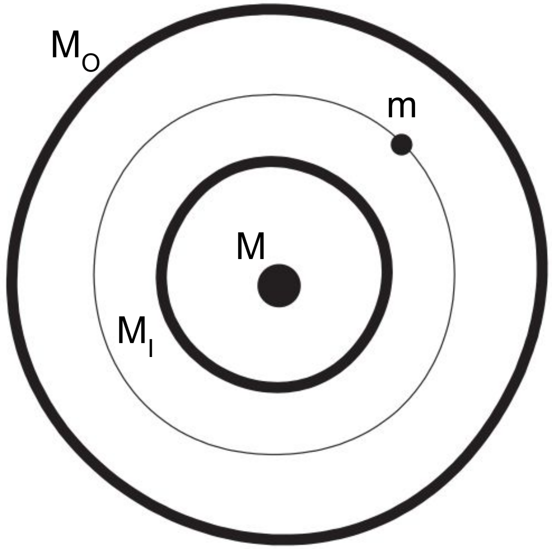
$$E_0[n_0] = \min_n (E[n])$$

Approximation 4: replace many-particle system with one particle system in effective potential

Reality:
The real orbit slightly wiggles due to many-particle interaction.



Mean-field approximation:
The orbit is calculated assuming that m rotates around one object with mass $M+M_I$



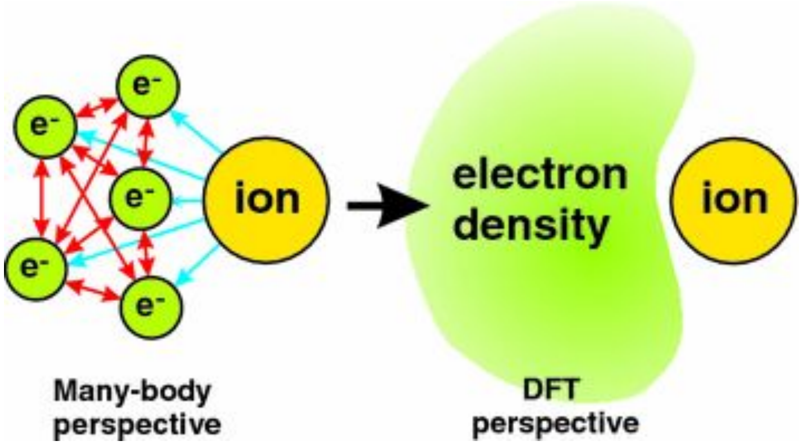
The wiggle due to many-particle interactions is called *correlation*

Approximation 4: Kohn - Sham theory

Replace the original interacting many-body system with an auxiliary one of non-interacting electrons. Take interaction into account with two terms:

1) Interaction of each electron with electron density (V_{Hartree})
2) Interaction of each electron with exchange-correlation potential (V_{XC})

Lu Jeu Sham



n
it is

Hohenberg-Kohn + Kohn-Sham

=

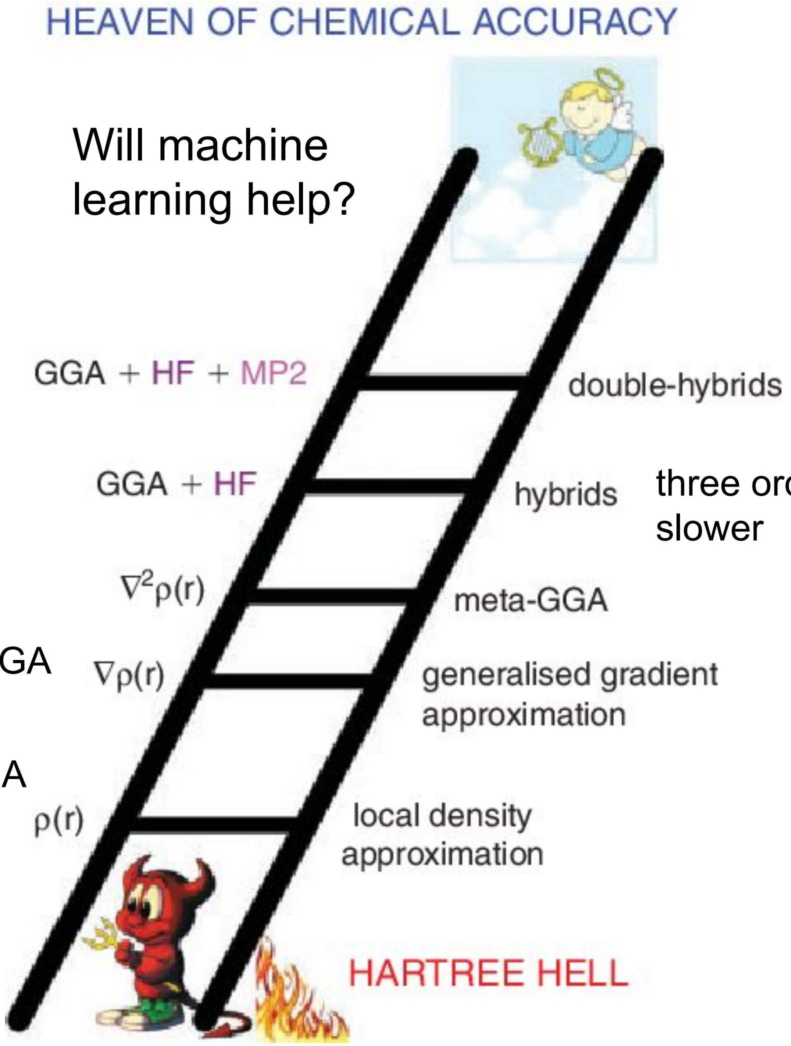
Density functional theory (DFT)

Rush for accurate exchange-correlation potential

$$V_{eff}(\mathbf{r}) = V_{ext}(\mathbf{r}) + V_{Hartree}[n] + V_{xc}[n]$$

In principle, if we can know the true form $\boldsymbol{V_{xc}[n]}$, we can have the exact solution of many-particle system

John P. Perdew, one of the developers of exchange correlation functionals made an analogy with **Jacob's Ladder** AIP Conference Proceedings 577, 1 (2001)



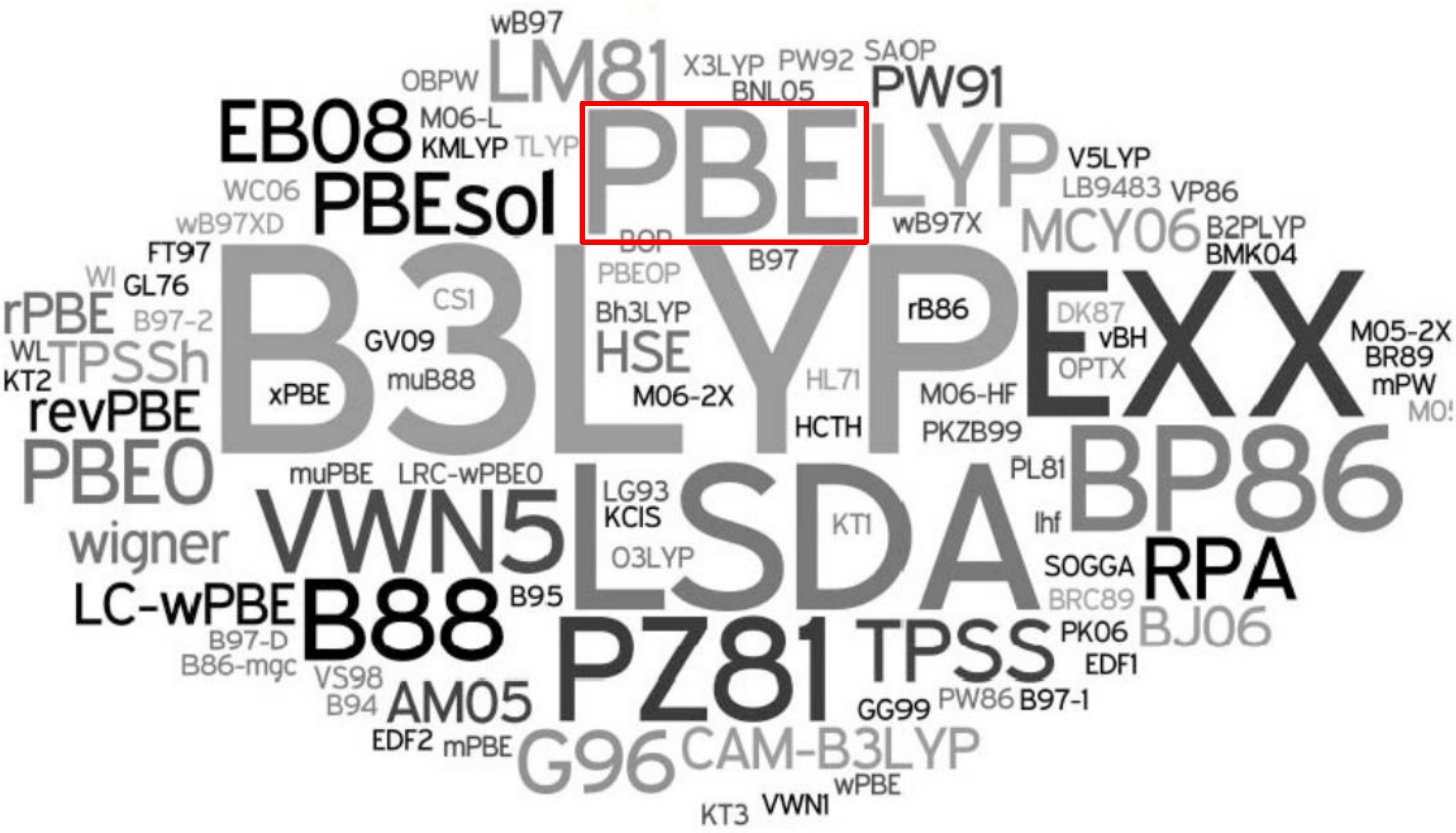
Will machine learning help?

three orders slower

GGA

LDA

Exchange-correlation functional flavours



Perdew, John P., Kieron **Burke**, and Matthias **Ernzerhof** Generalized gradient approximation made simple, *Phys. Rev. Let.* 77 (1996) 3865

138 000 citations in 2019, 202 000 in 2024!

Summary of approximations used in DFT

- 👌Born-Oppenheimer approximation - decouple electron and nuclei dynamics
  - very accurate for ground state properties - lattice constants, energies, elastic, etc.
- 👌Total energy and other properties as a functional of electronic density
  - not an approximation at al, just equivalent description
- 👌Pseudopotential for core electrons
  - very accurate for chemical tasks
- 📛One many-electron system ⇒ many one-electron systems with effective potential;
  - Many-electron effects are inside exchange-correlation potential (V_{XC})
  - In principle can be exact, but exact V_{XC} is unknown,
  - V_{XC} is approximated with several levels of accuracy, but the receipt for systematic improvement is still unknown!
  - The main source of errors in DFT calculations. Binding energies of molecules, band gaps, surfaces and strongly-correlated systems are especially sensitive to V_{XC}

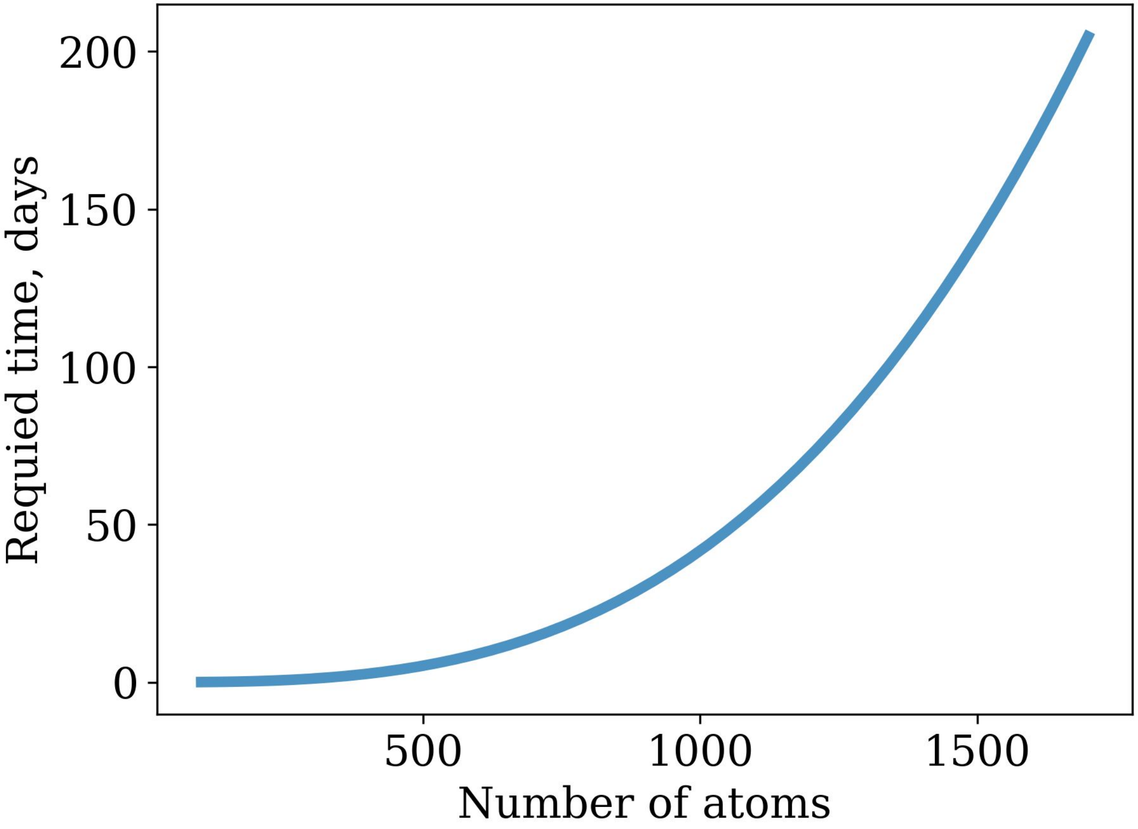
What can be calculated with DFT for solids?

In principle everything!

In practice it is limited by the complexity (size) of a system:

- The computer time required grow as n^3, where n is number of electrons.

- E.g. on a 16-core modern processor, 1000 electrons (100 Ni atoms), one calculation of total energy requires from 20 min to 1 hour

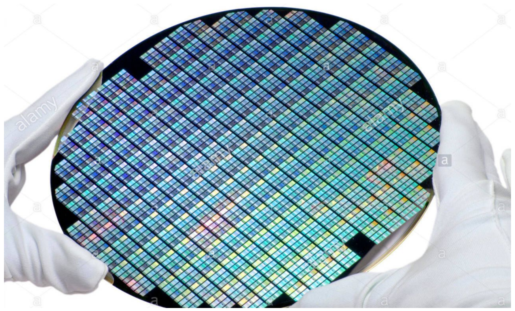


But solids contain in the order of one mole of matter 10^{23} atoms!
How they can be treated computationally?

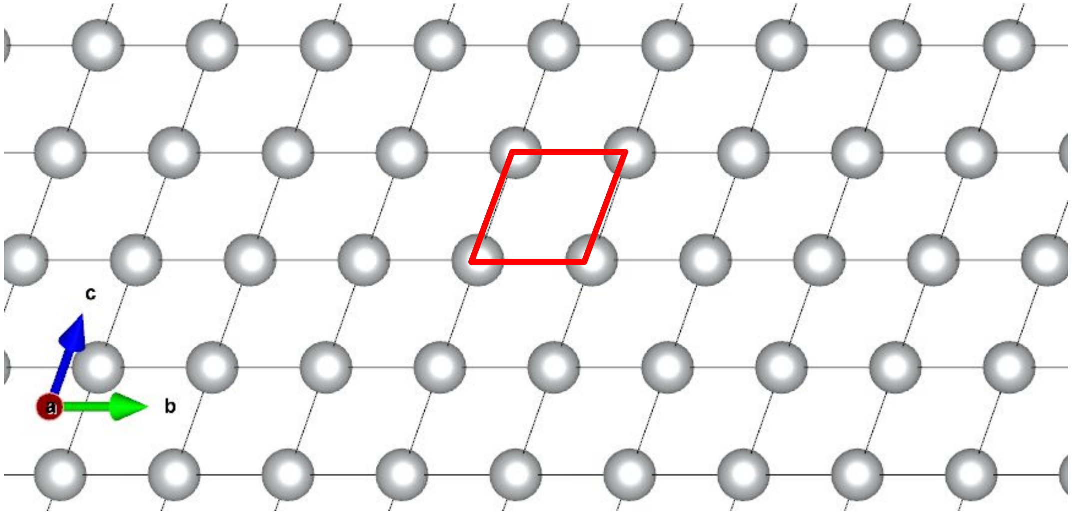
Periodicity of crystals

Insulators

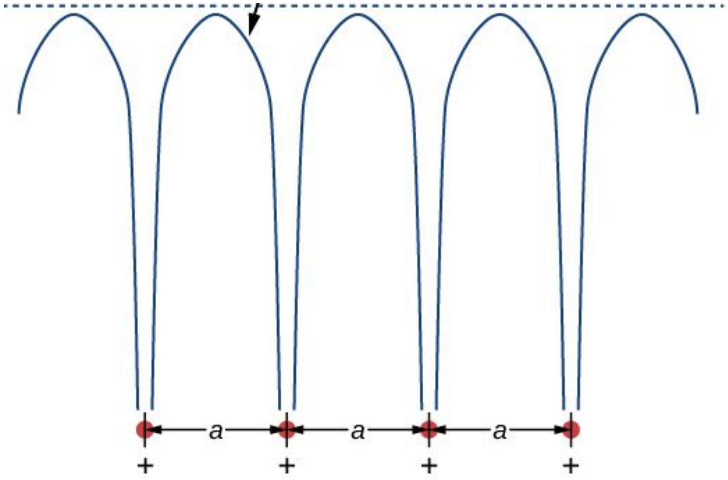
Semiconductors



Metals and alloys



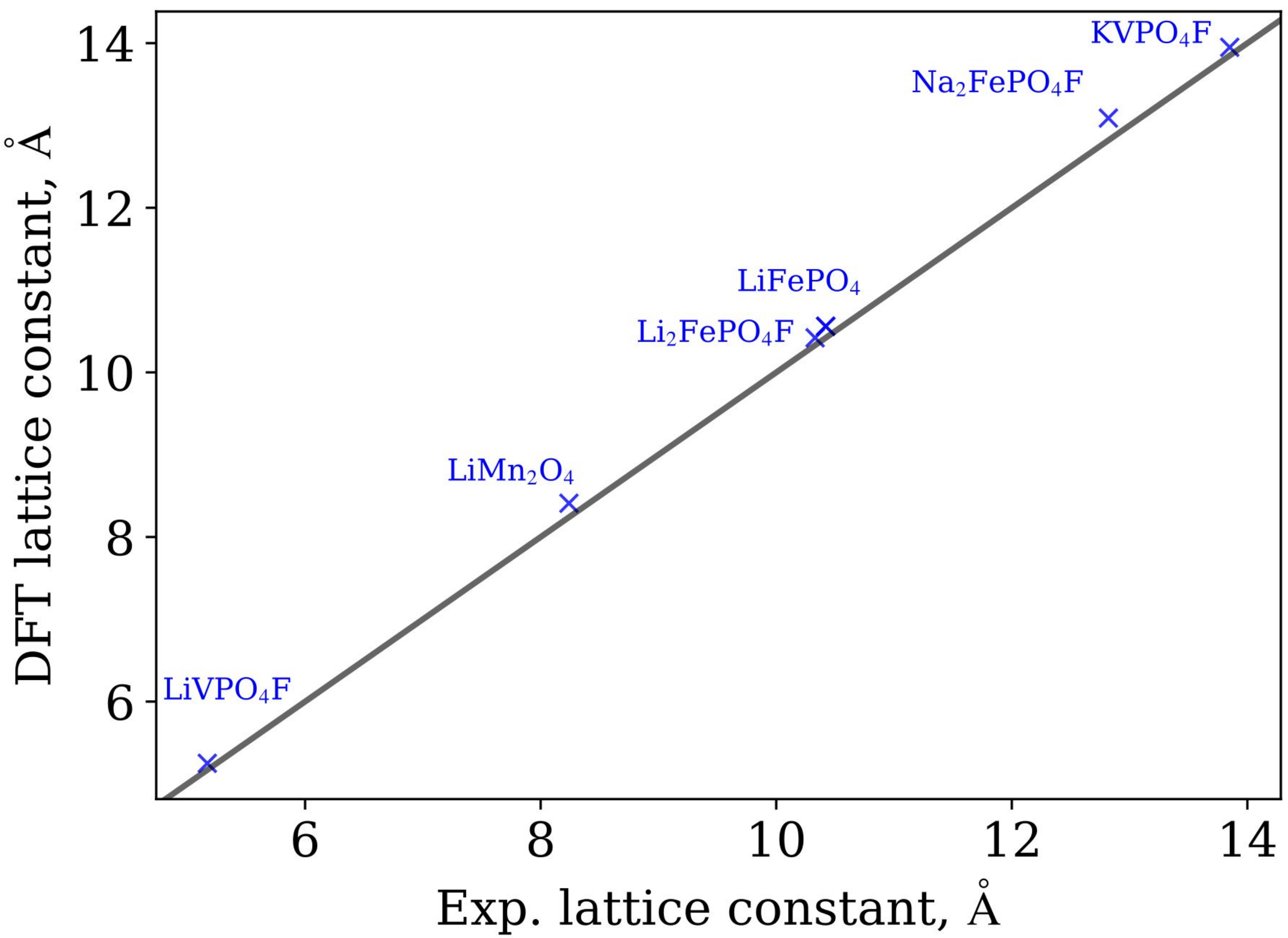
Potential and wave function are periodic therefore only one unit cell can be treated computationally. It is easily realized in DFT



Li - 1 atom, $LiCoO_2$ - 4 atoms, $Li_7La_3Zr_2O_{12}$ - **96 atoms**!

Accuracy?

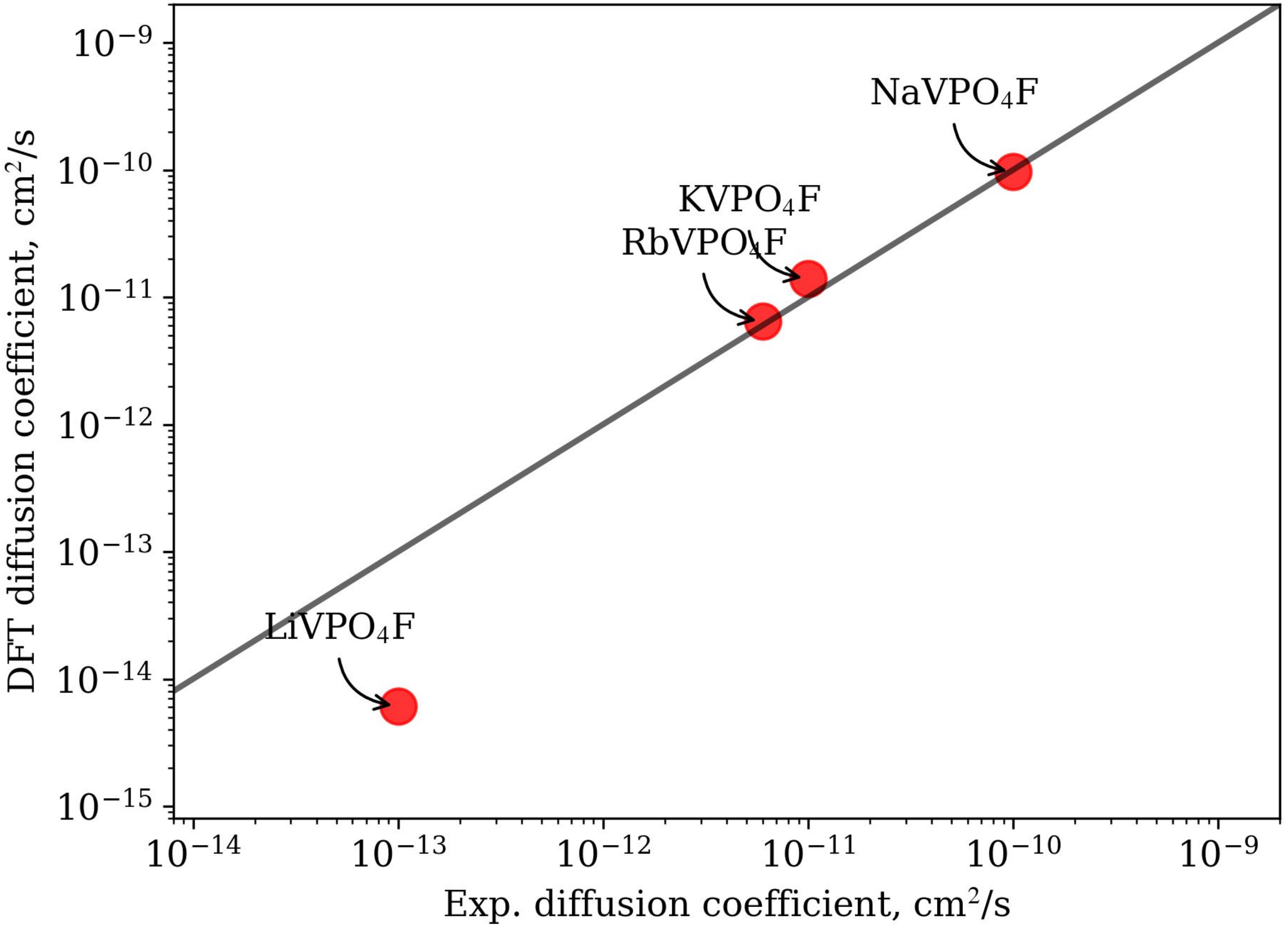
Accuracy: Lattice constants (**1-2%** overestimation)



Vanadyl bond length in NaVOPO4 is overestimated by 5% in PBE+U, but hybrid functional is accurate (<1%)

Aksyonov, *Comp. Mat. Sci.* 154 (2018) 449–458

DFT vs Experiment (KTP structures)



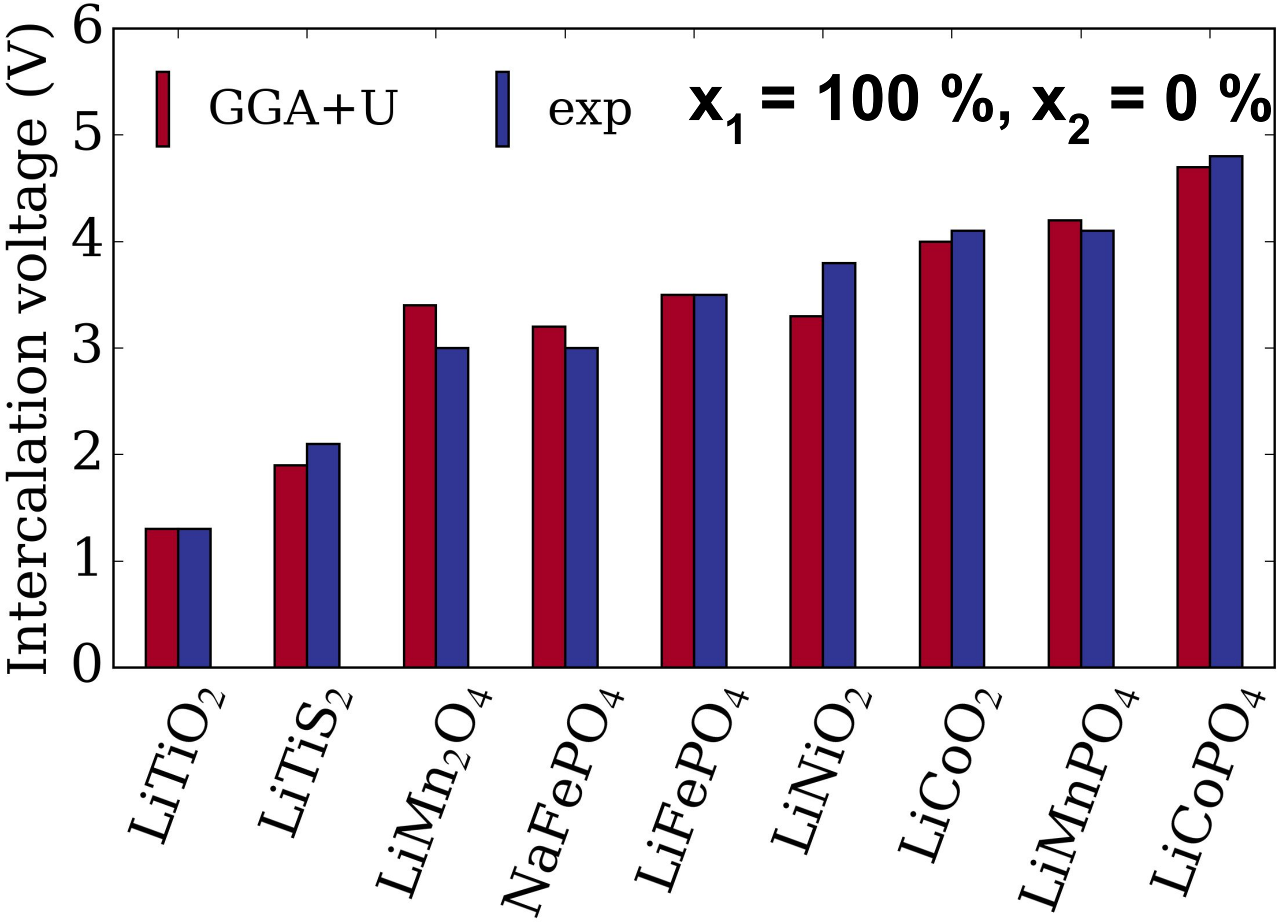
$$D(T) \approx D_0 \ e^{-\frac{E_a}{k_B T}},$$

pre-exponential factor?

Nat. comm. 2022, 13, 4097
J. Mater. Chem. A, 2018, 6, 14420–14430
J. Electr. Soc., 2017, 164, A6373-A6380

Total energy example: Intercalation potentials

$$\overline{V}(x_1, x_2) \approx -\frac{E(\mathrm{Li}_{x_1}\mathrm{MO}_2) - E(\mathrm{Li}_{x_2}\mathrm{MO}_2) - (x_1 - x_2)\, E(\mathrm{Li})}{(x_1 - x_2)\, F}$$



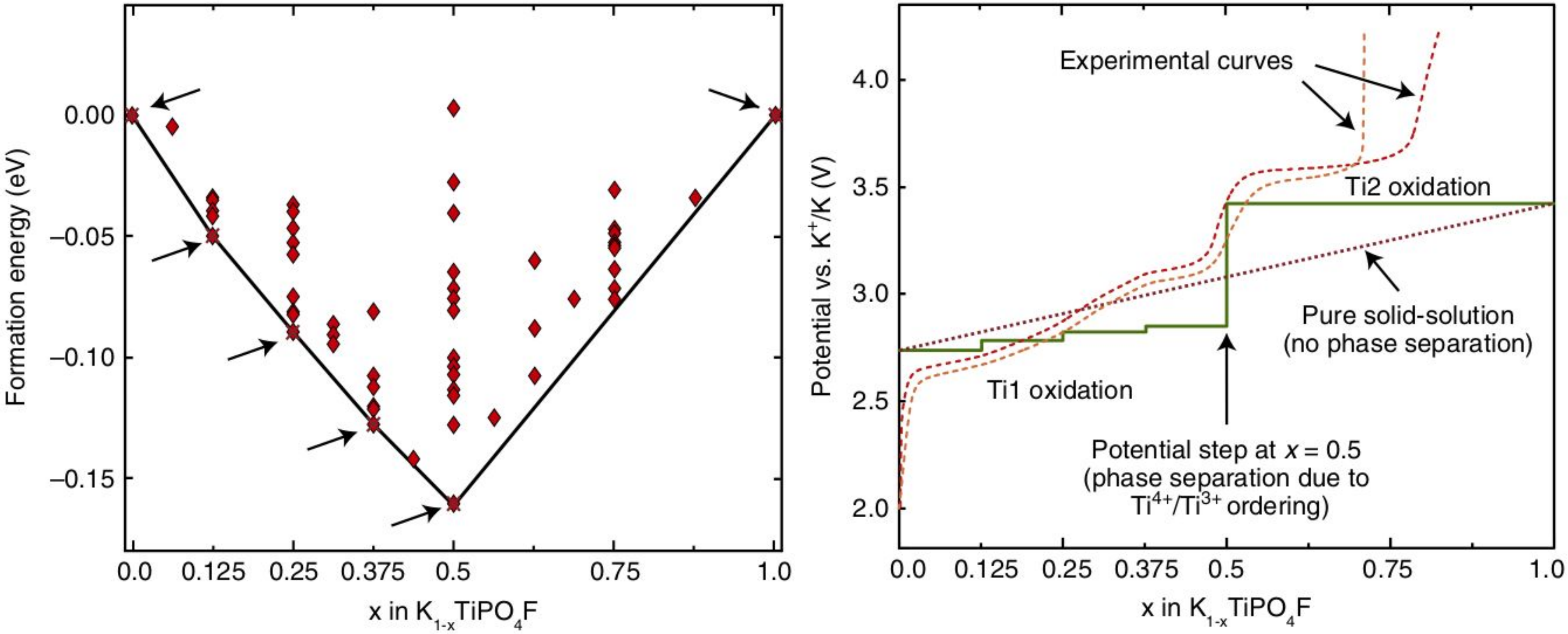
$x_1 = 100\ \%$, $x_2 = 0\ \%$

DFT+U is required
The U value can be determined self-consistently from first-principles. However, oftenly it is fitted to experimental data

Another option is to use hybrid functionals, but in this case the calculation time increases by 3 orders of magnitude for plane-wave DFT codes

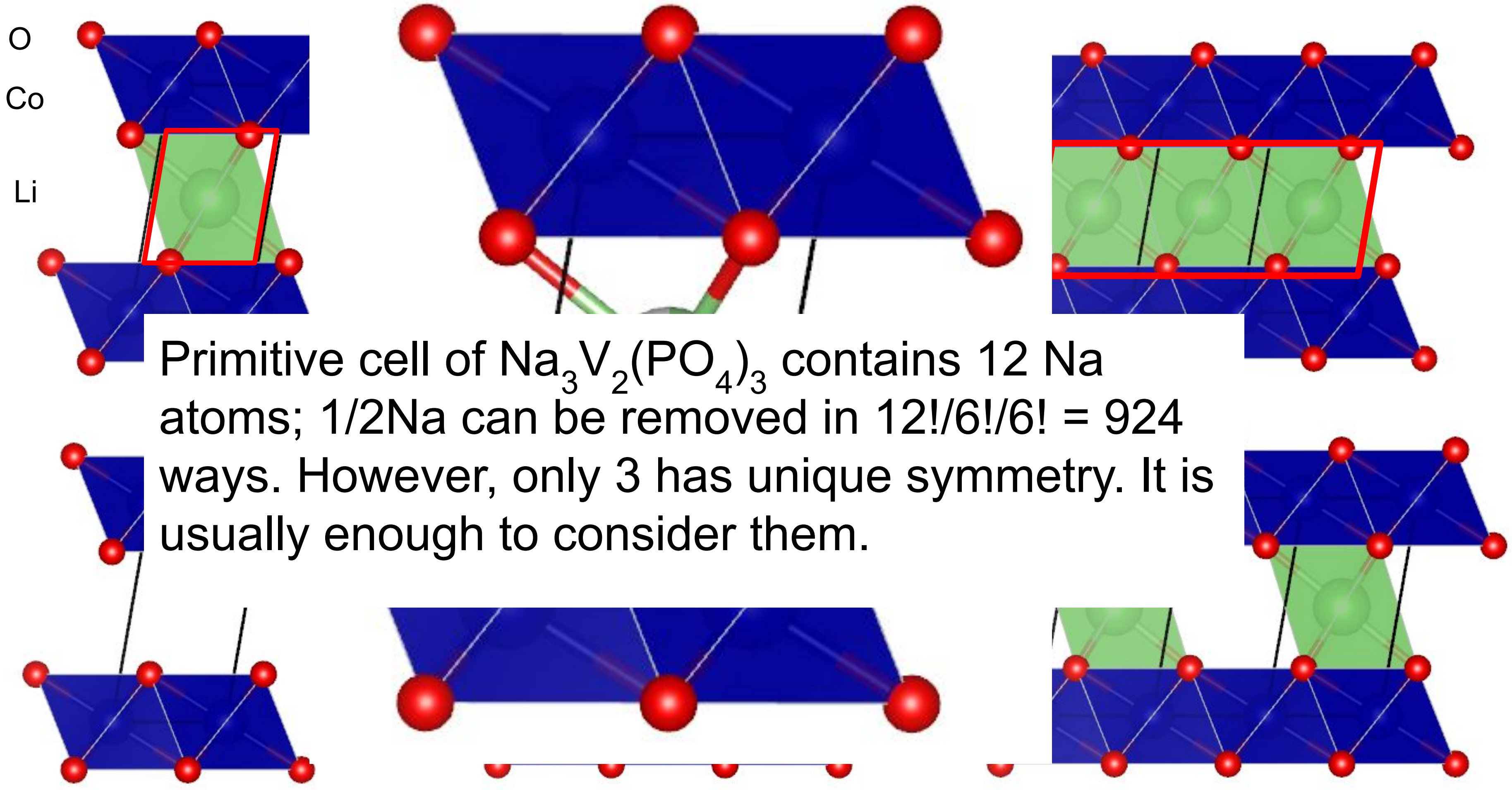
Total energy example: phase diagrams, voltage profile

How to calculate phases with intermediate concentrations?



Fedotov et al., *Nat. Comm.* 11 (2020) 1484

Intermediate concentrations: construct supercells

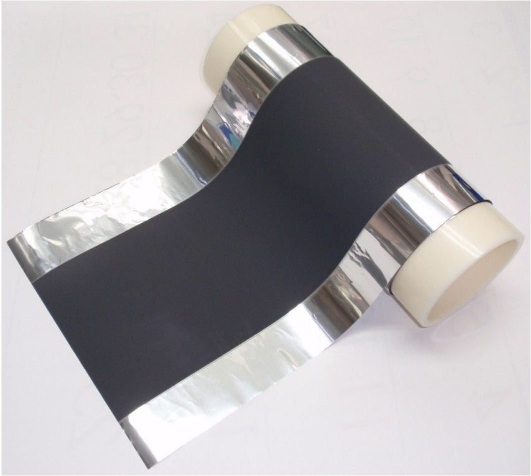


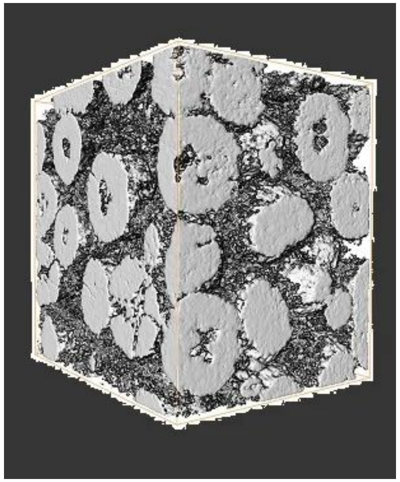
Primitive cell of $Na_3V_2(PO_4)_3$ contains 12 Na atoms; 1/2Na can be removed in 12!/6!/6! = 924 ways. However, only 3 has unique symmetry. It is usually enough to consider them.

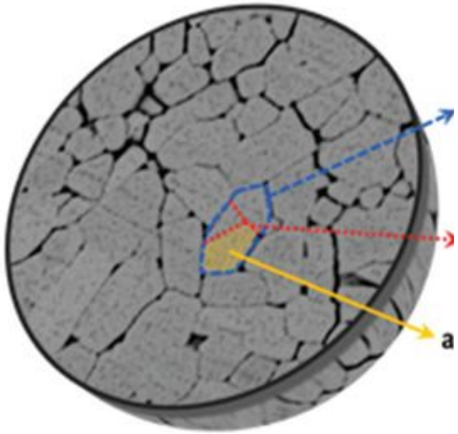
$LiCoO_2 \rightarrow CoO_2$ $LiCoO_2 \rightarrow Li_{1/2}CoO_2$ $LiCoO_2 \rightarrow Li_{1/3}CoO_2$

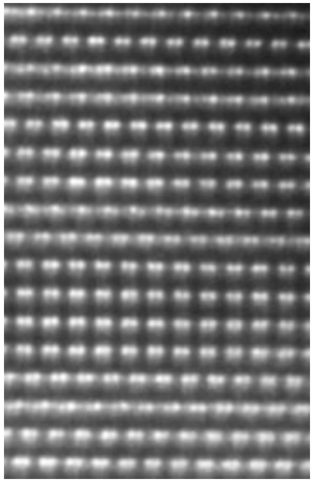
Connection to real materials

- Using one primitive cell an infinite ideal crystal can be modelled allowing to consider numerous properties
  - crystal structure and lattice constants
  - energy phase stability
  - electronic structure and functional properties
- By choosing an appropriate functional very good agreement between theory and experiment can be obtained (within several percents)
- However, one should always keep in mind that real materials are far from ideal



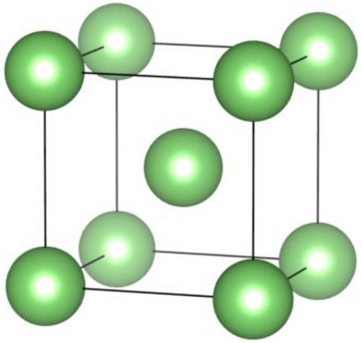




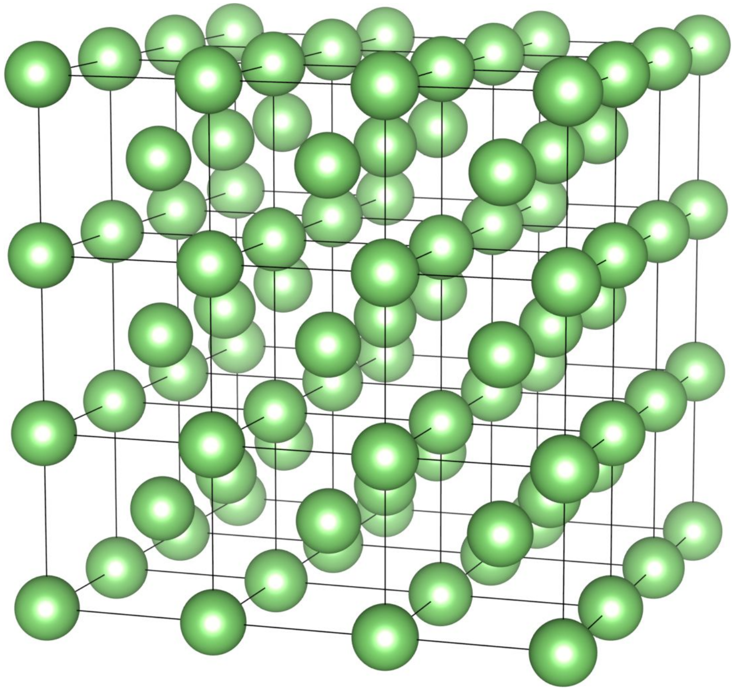


Modeling of defects: vacancies

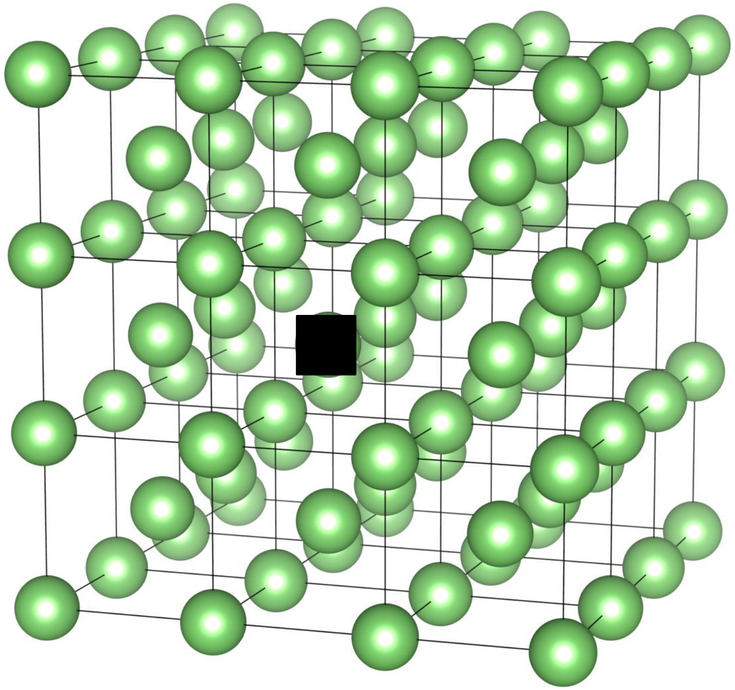
DFT allows modeling of complex defects
Once you can insulate the role of some defect you can study it with DFT modeling



BCC unit cell



3x3 supercell

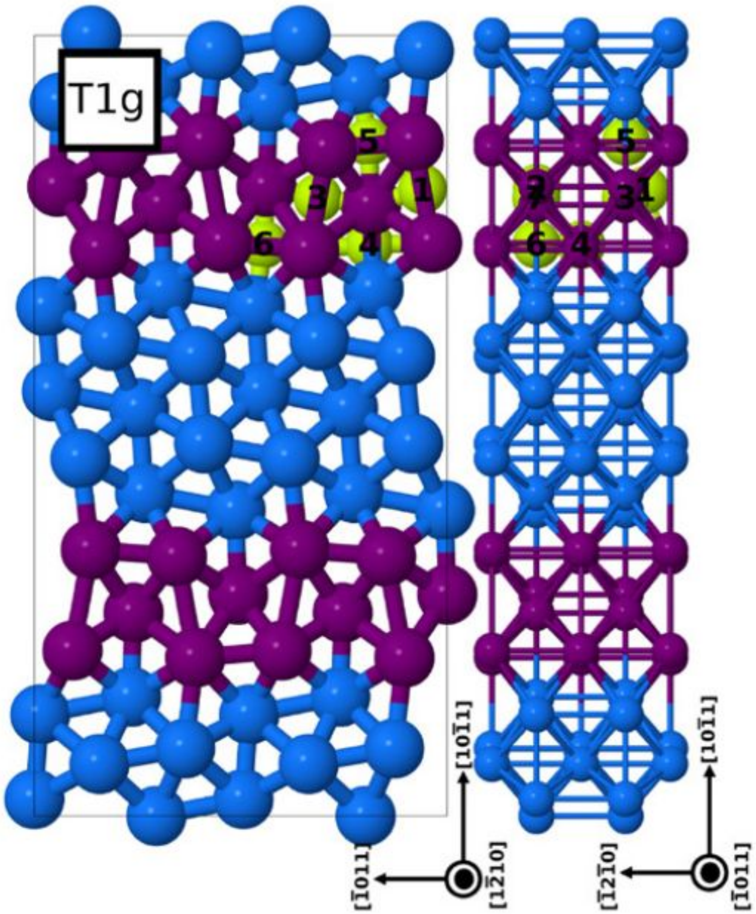


3x3 supercell with vacancy

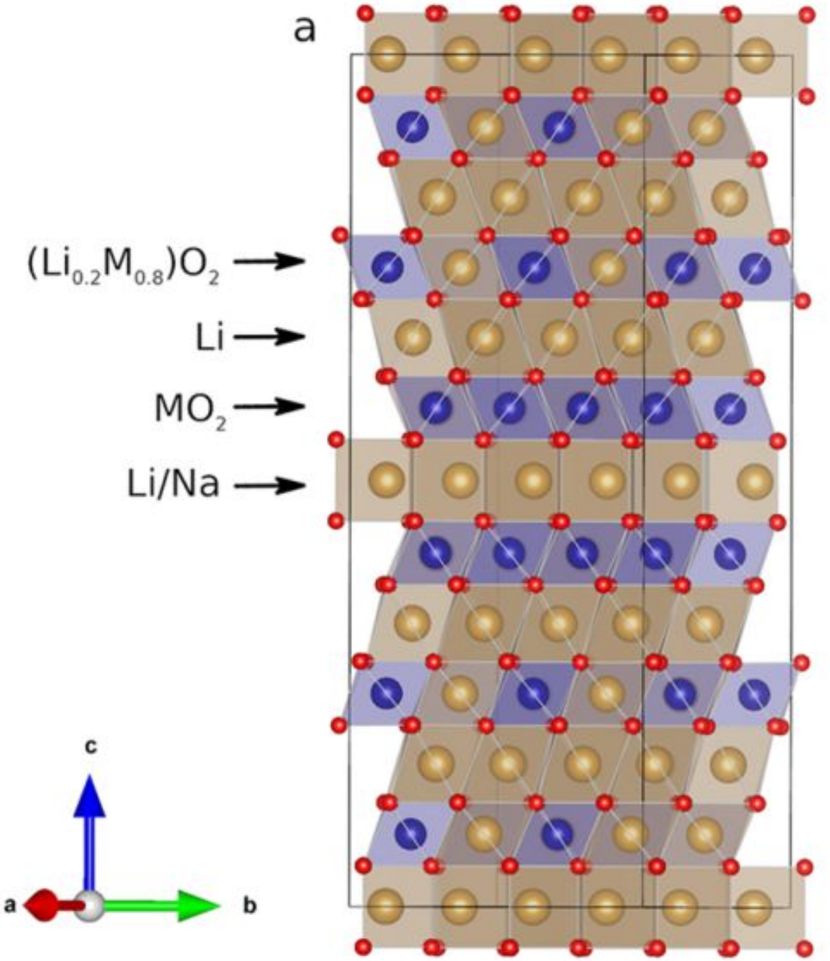
A vacancy is repeated every third unit cell infinitely -> so we have matrix of vacancies
If the distance is large enough vacancies don’t know about each other and don’t interact
10x10x10 A is usually enough

Modeling of defects: grain boundaries

hcp Titanium:

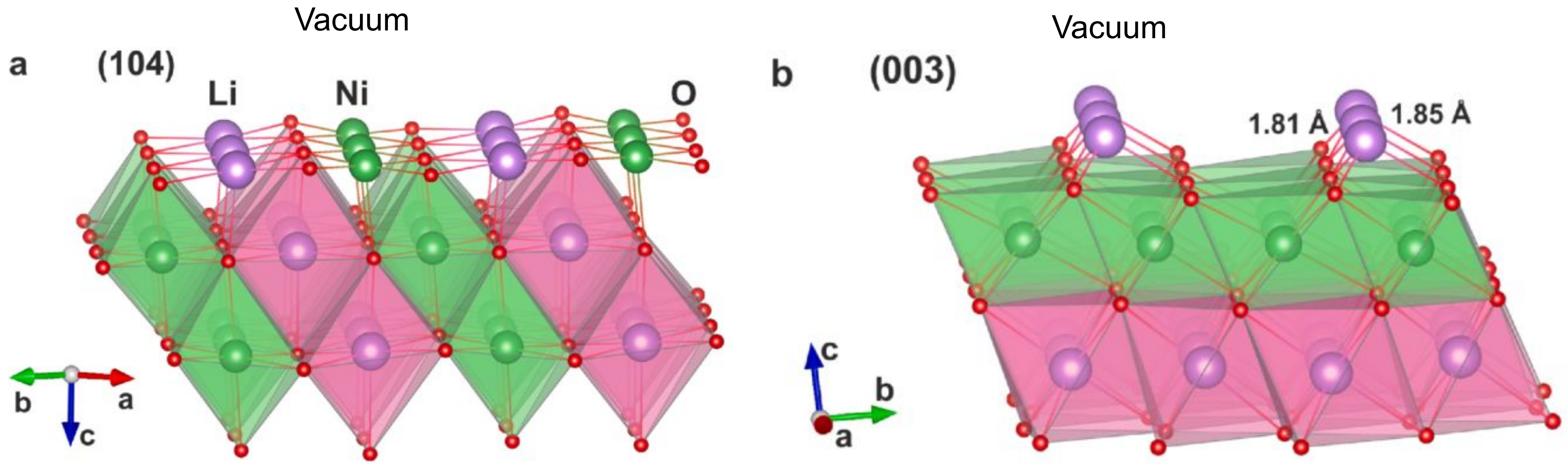


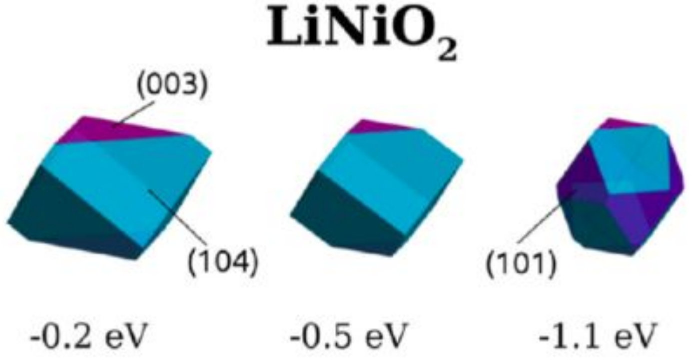
Aksyonov et al. J. Phys.: Condens. Matter 28 (2016) 385001



Abakumov et al. ACS Appl. Energy Mater. 2021, 4, 6777−6786

Modeling of defects: surfaces





Structure (can be difficult) and energetics of defects

Influence on

- mechanical strength
- diffusion characteristics
- morphology of particles

A.O. Boev, et al. Applied Surface Science 537 (2021) 147750

Conductivity based on 0 K migration barriers

Nernst–Einstein relation for ionic conductivity. N_{Li} is the number of lithium ions, V is the volume of the simulation cell

$$\sigma(T) = \frac{N_{\mathrm{Li}} \; e^2}{V \; k_B \; T} \, D(T),$$

Diffusion is

$$D(T) \approx D_0 \; e^{-\frac{E_a}{k_B T}},$$

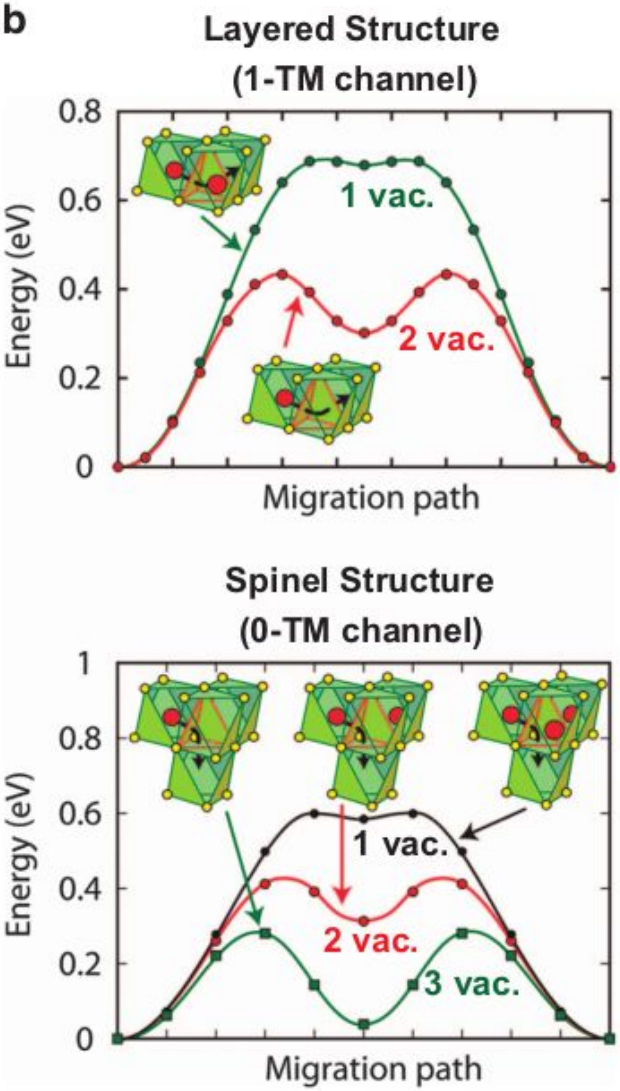
$$D_0 = g a^2 v^*,$$

g is geometrical factor (~1)

a is hopping distance,

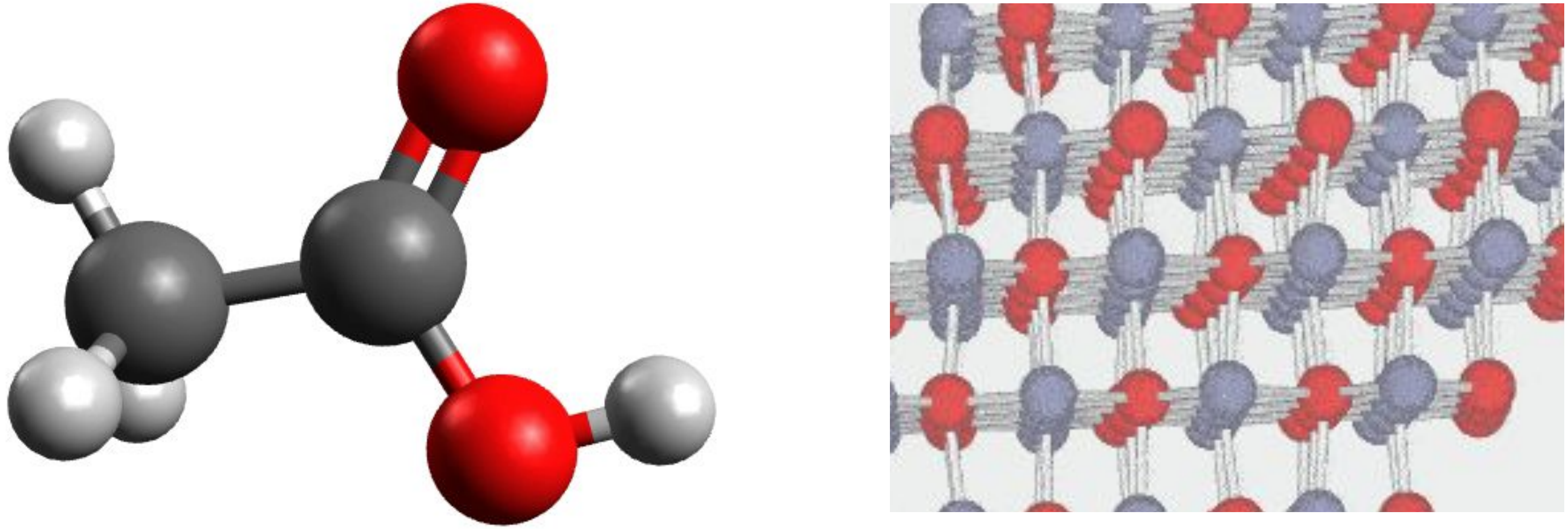
v^* is temperature-independent effective attempt frequency (10^{11} to 10^{13}),

E_a is migration barrier



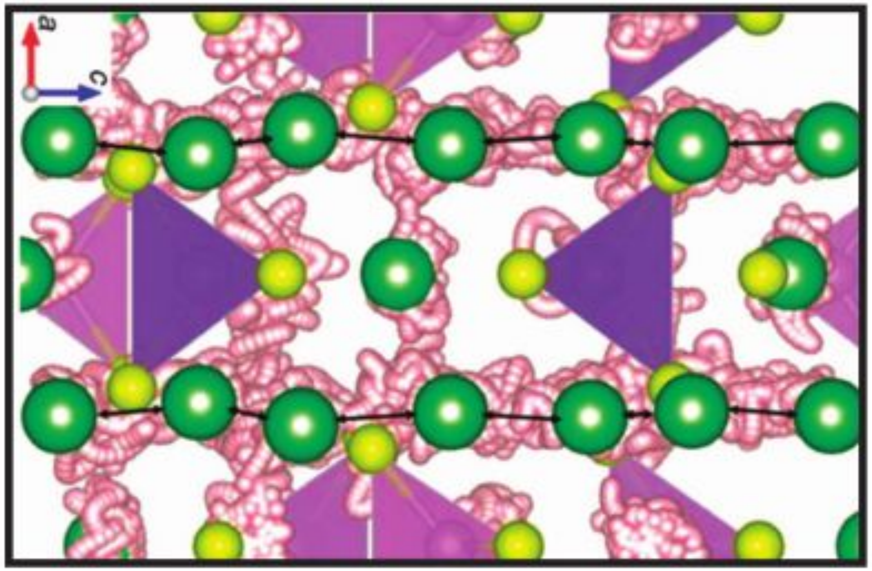
Crystal lattice dynamics

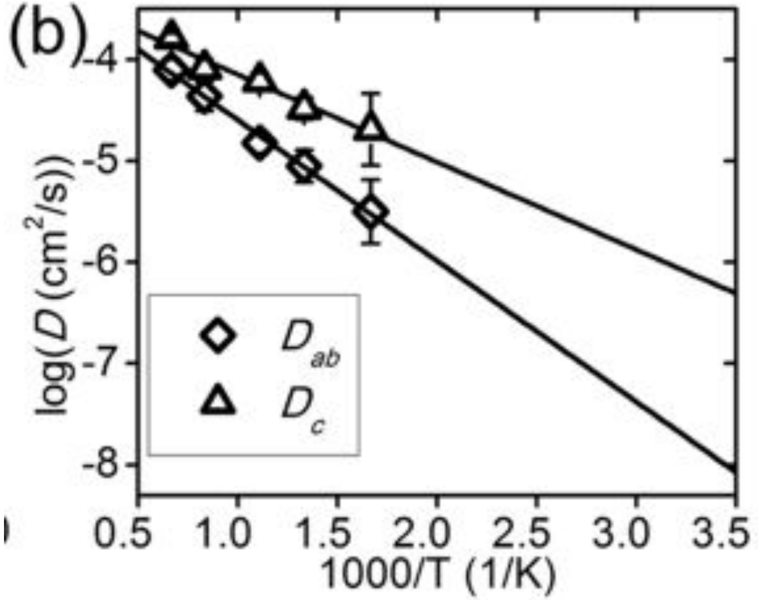
Even at zero T atoms have zero-point T vibrations. At higher temperatures the vibrations increases. Collective modes are known as phonons



- By taking into account vibration, the impact of temperature can be studied

Ionic conductivity, *Ab initio* MD





Li trajectories in $Li_{10}GeP_2S_{12}$ at 900 K

$$D(T) \approx D_0 \; e^{-\frac{E_a}{k_B T}},$$

Can be used to simulate diffusion of transition metals during sintering

Mo, Yifei, Shyue Ping Ong, and Gerbrand Ceder. " *Chemistry of Materials* 24.1 (2012): 15-17.

Urban, A. et al.// *npj Computational Materials* 2.1 (2016): 1-13.

Summary of crystal modeling

- By considering only one unit cell an infinite ideal crystal can be modelled
- The structure and almost all crystal properties can be calculated: mechanical, electric, magnetic, etc. with very good accuracy (1-10%)
- Real crystals with defects can be modeled using supercell approach.
- By a wise selection of model systems very complex phenomena in crystal can be considered
- The effects of temperature are taken into account with the help by calculating collective migrations, known as phonons, and Molecular Dynamics

Sources

1. J. Garcia et al. / Chem. Mater. 2020, 32, 9126−9139 - $MnCO_3$ co-precipitation modeling
2. A. Moitra et al. / Acta Materialia 58 (2010) 3939–3951 - W sintering modeling

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