HPC SCHOOL ON QUANTUM COMPUTATIONAL MATERIALS SCIENCE

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Institut des sciences du calcul et des données
SORBONNE UNIVERSITÉ

A. Marco Saitta

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie – Sorbonne U, CNRS, MNHN

Introduction to Computational Materials Science in Sorbonne: from DFT to machine learning methods

Paris/Singapore, Nov 17th 2020

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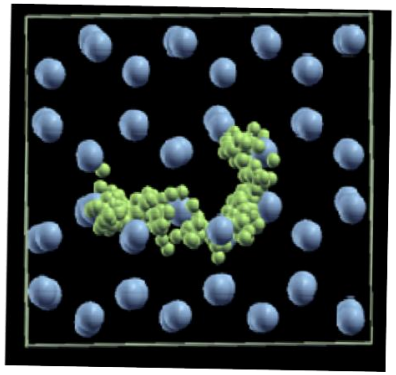

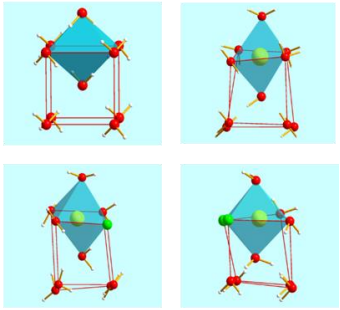

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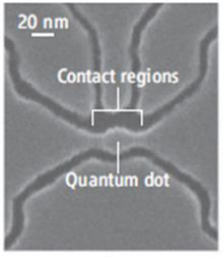

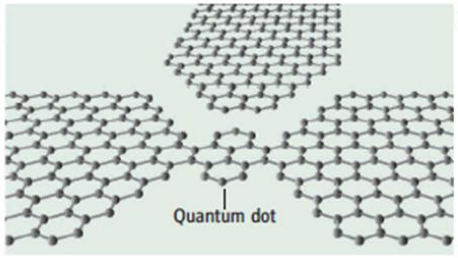

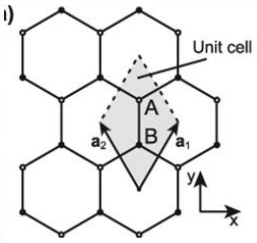

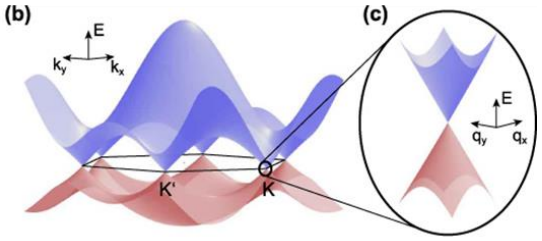

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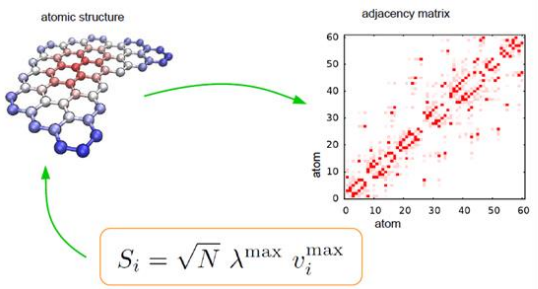
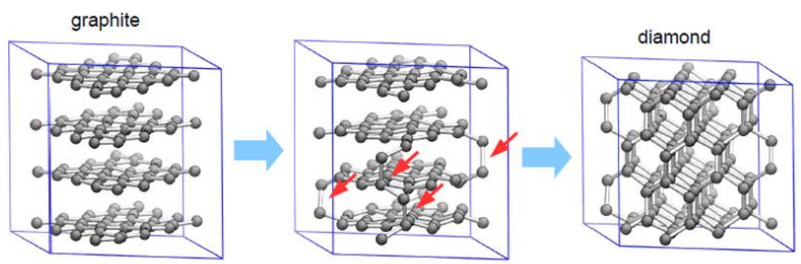
  - Topology-based theory of transformations of matter (MAESTRO)

MAESTRO





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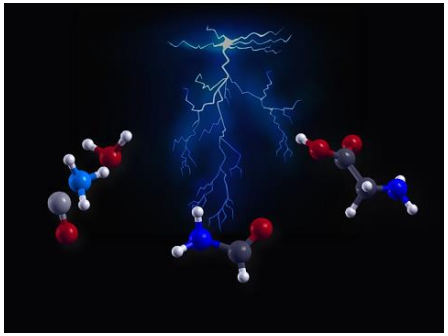
  - Physical origins of biological life (NASA)

NASA Goddard



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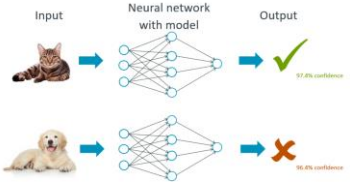
  - Machine-learning methods in computational materials science



scai
SORBONNE CENTER FOR ARTIFICIAL INTELLIGENCE

Paris International School on Advanced Computational Materials Science

PISACMS

A. Marco SAITTA – Rodolphe VUILLEUMIER

Why

- Sorbonne: a singular generation of computational physicists and chemists working together
- Method development over the whole scale: from hydrodynamics models to Quantum MonteCarlo
- Strong support from our institutions; availability of computer labs
- Share our knowledge and pass it to new generations of computational physicists and chemists; help build new connections

What

- Classical Molecular Dynamics
- Density Functional Theory
- Ab Initio Molecular Dynamics
- Advanced Coarse-Graining and Mesoscale Methods
- Metadynamics & Free Energy Methods
- Density Functional Perturbation Theory
- Path-Integral Methods
- Classical & Quantum Monte-Carlo
- Machine Learning methods

Who

- Michele CASULA – IMPMC (Physics)
- Marie JARDAT – PHENIX (Chemistry)
- Maximilien LEVESQUE – PASTEUR (Chemistry)
- Michele LAZZERI – IMPMC (Physics)
- Virginie MARRY – PHENIX (Chemistry)
- Fabio PIETRUCCI – IMPMC (Physics)
- Benjamin ROTENBERG – PHENIX (Chemistry)
- A. Marco SAITTA – IMPMC (Physics)
- Mathieu SALANNE – PHENIX (Chemistry)
- Ari SEITSONEN – PASTEUR (Chemistry)
- Rodolphe VUILLEUMIER – PASTEUR (Chemistry)

When & where

- Paris 2015: Aug 24 – Aug 28, UPMC Campus
- Paris 2016: Aug 29 – Sept 2, UPMC Campus
- Paris 2017: Aug 28 – Sept 1, UPMC Campus
- Bangalore 2018: joint SU-JNCASR « SJSACMS »
- Paris 2018: Aug 27 – Aug 31, SU PMC Campus
- Paris 2019: Aug 26 – Aug 30, SU PMC Campus
- Paris 2020: Aug 24 – Aug 28, SU PMC Campus
- Singapore 2020: Nov 16 – Nov 20, NUS Campus
- Paris 2021
- Singapore 2021
- Abu Dhabi 2022 ?
- Bangalore 2022 ?

http://pisacms.sciencesconf.org

MAterials for Energy through STochastic sampling and high peRformance cOmputing

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Team members

- Michele CASULA – IMPMC (Physics)
- Julien BIGOT – CEA (Computer Science)
- Ludovic GOUDENEGE – CentraleSupélec (Mathematics)
- Guillaume JOSLIN – CentraleSupélec (Computer Science)
- Pierre MONMARCHE – LJLL/LCT (Mathematics/Chemistry)
- Fabio PIETRUCCI – IMPMC (Physics)
- Benjamin ROTENBERG – PHENIX (Chemistry)
- **A. Marco SAITTA – IMPMC (Physics)**
- Mathieu SALANNE – PHENIX (Chemistry)
- Rodolphe VUILLEUMIER – PASTEUR (Chemistry)

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Main Research Lines

- **Maths/Physics (WP1)**
  - Dimensionality reduction/coordinate optimization

- **Physics/Chemistry (WP2)**
  - (Energy-storage-interesting) ionic salts in solution

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A general overview of our scientific interests (with Fabio Pietrucci)

- What: "generalized" structural transformations in condensed matter physics and chemistry
  - Phase transitions (under pressure)
  - Nucleation from the liquid phase
  - Chemical reactions in solutions
  - Protein structure-function relations
- How: computer simulations of *ab initio* (= quantum) molecular dynamics
- One emblematic case: CO_2 at "geological" conditions
- Bottleneck: efficient sampling of 3N-dimensional configurational space
- Challenge n.1 : find "good" collective variables to describe/project the manifold onto a few relevant dimensions
- Challenge n.2 : replace costly ab initio simulations by machine-learning-based ones

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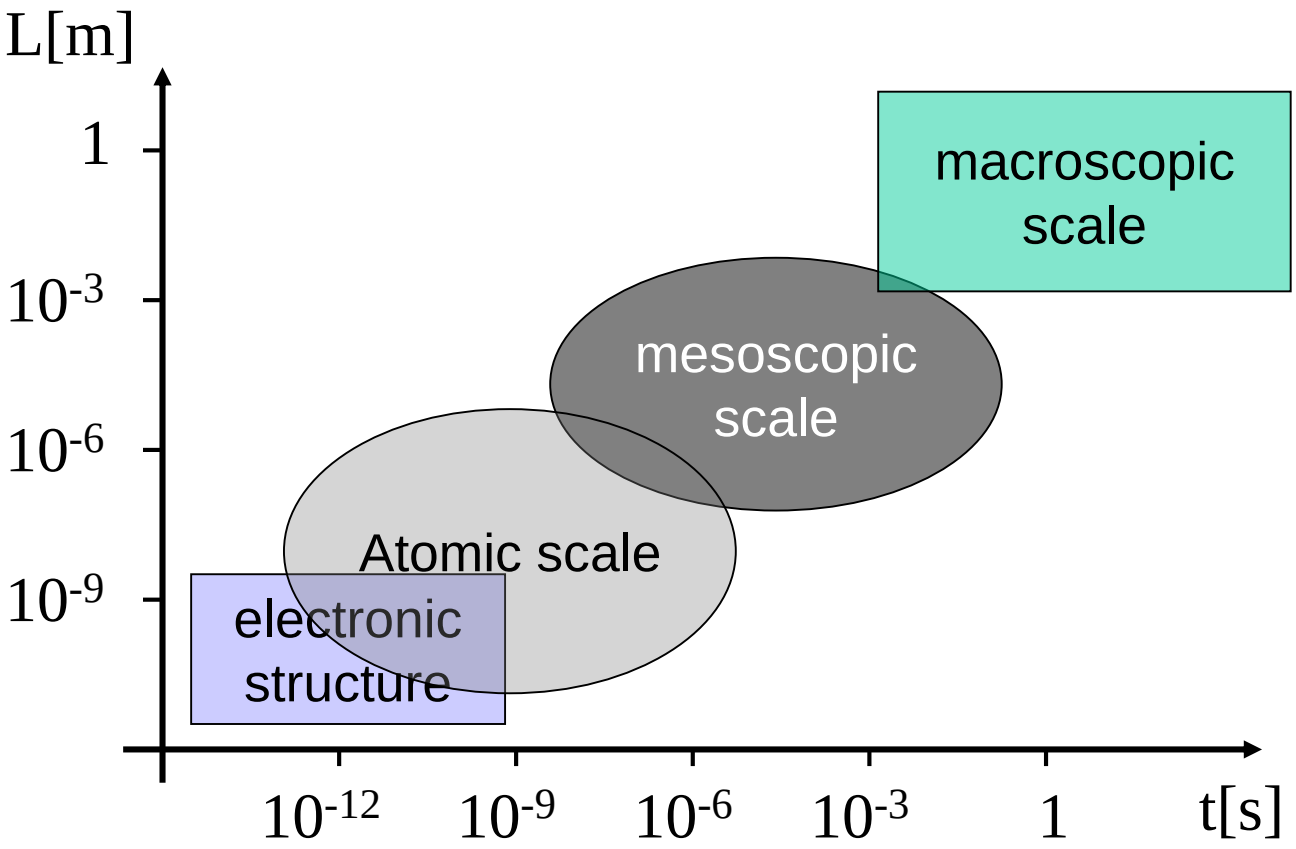
Length/time scales, methods



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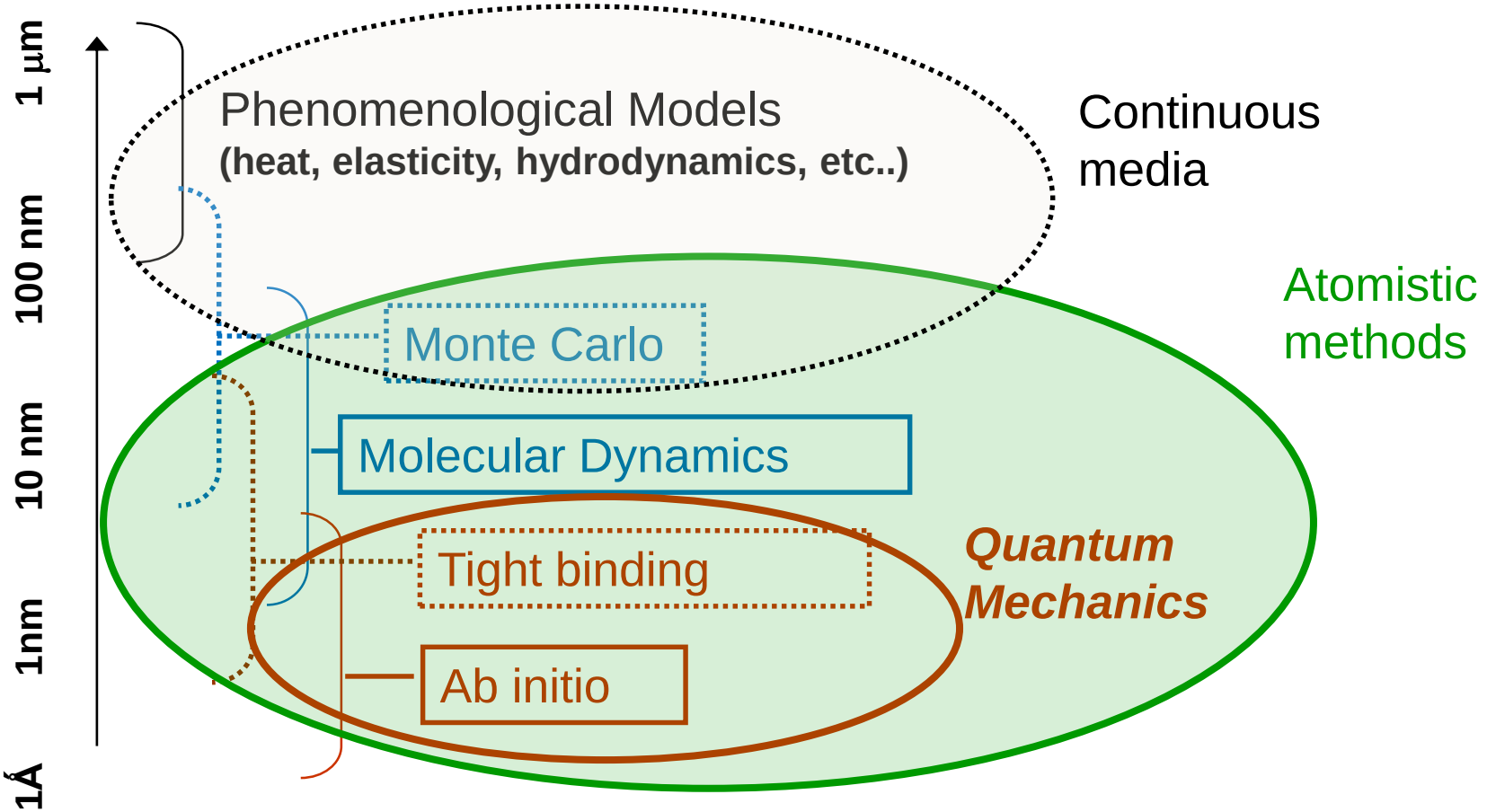

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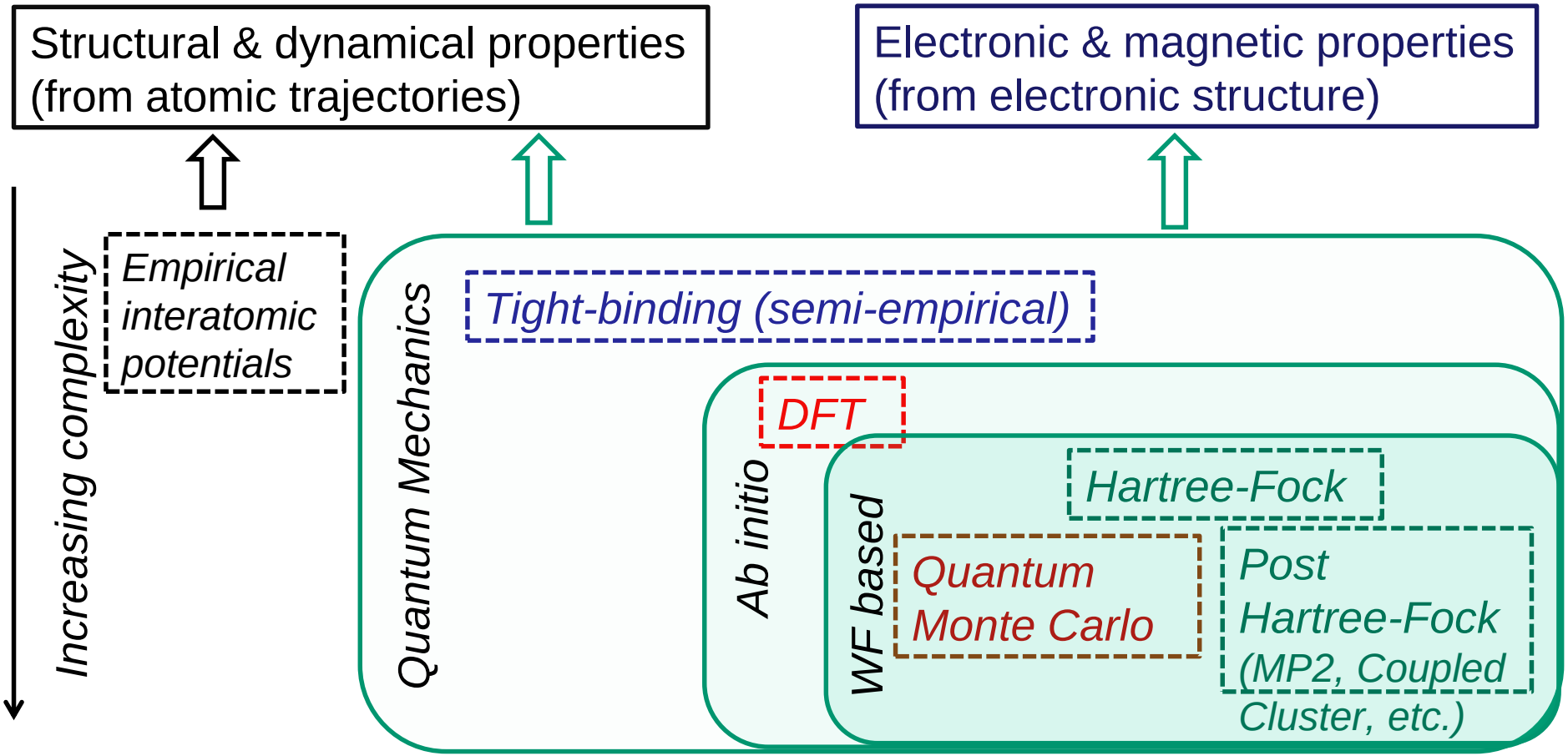


Ab initio DFT calculations

- *Ab initio* interactions solely determined by the electronic structure of atoms
- Solution of the quantum mechanical EOM of the electrons: energy and forces
- Atomic number the only "external" input: transferability
- However, a special theoretical framework is needed

Ab initio DFT calculations

- Same approach from biology to planet interiors
- Electronic structure and properties, chemical reactions, change of coordination
- Accuracy at the (sub)nano scale
- Directly simulate experimental spectra (x-ray, Raman, infrared, NMR,…)

Ab initio DFT calculations

Generality (« transferability »): all atoms from periodic table
Desired accuracy (« predictive » theory):

- cristallographic positions ± 0.005 Å
- bonding energies ± 40 meV/atom (≅ 1 kcal/mol)
- vibrational frequences 100 GHz ~ 3.3 cm^{-1}
- dipolar moments ± 0.02 D
- magnetic moments ± 0.1 μ_B
- spectra (visible, UV, X) ± 0.1 eV

Typical system size: < 10^3 atoms

Typical time scale: ~ 10^{-11} s

Computational efficiency: parallel algorithms, modularity

The many-electron problem

Time-independent, non-relativistic, spinless, Schrödinger equation for N electrons interacting with fixed nuclei

$$H\Psi(\vec{r}_1,\ldots,\vec{r}_N) = \varepsilon\Psi(\vec{r}_1,\ldots,\vec{r}_N)$$

$$H = \sum_{i=1}^{N}\left[-\frac{\hbar^2\nabla_i^2}{2m} + V_{\text{ext}}(\vec{r}_i)\right] + \sum_{i>j}\frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

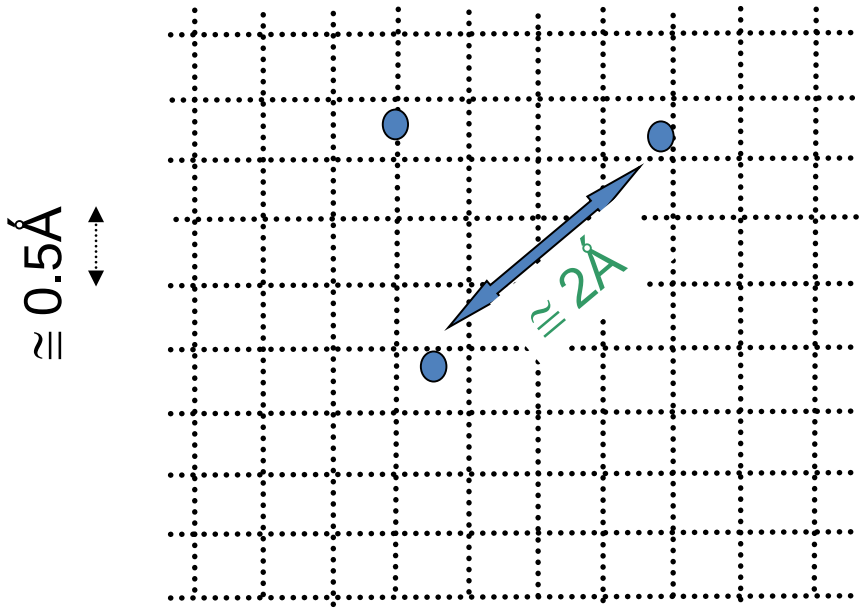
sum of *N* one-electron operators (kinetic operator + Coulomb potential from the nuclei)

Long range e^- – e^- interaction (the big problem!)

Can we solve it numerically by brute force?

The many-electron problem by brute force?

Example: Li_3 cluster



9 electrons

Solve the Schrödinger equation on a MxMxM grid <u>for each spatial coordinate</u>

For M=10 → 10^{27} x 2^9 independent variables

→ ~ 5 x 10^{29} operations just to evaluate $\langle \Psi | H | \Psi \rangle$!

On a Tflops computer this would need ~ 10^{11} years!
(unfeasible even if computer speed increases by a factor ~4 every ~2 yrs)

Adiabatic (Born-Oppenheimer) approximation

- Electrons much lighter & faster than nuclei, their timescales much shorter
- Quantum EOM for electrons, classical ones for ions
- Solution of the electrons QM: global many-body wavefunction, whose size grows exponentially

The electronic density

$$n(\vec{r}) = \langle\Psi|\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}_i)|\Psi\rangle = N\int d^3r_2\ldots\int d^3r_N\ |\Psi(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)|^2$$

- Is a function of 3 spatial coordinates, independently of N
- Is measurable
- Many physical quantities can be inferred from it

Can we reformulate the many-body electron problem in terms of *n(r)*?

The energy functional

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2 \nabla_i^2}{2m} + V_{\text{ext}}(\vec{r}_i) \right] + \sum_{i>j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

$$E[n] = T[n] + E_{\text{ext}}[n] + U[n]$$

$$E_{\text{ext}}[n] = \int d^3r \, V_{\text{ext}}(\vec{r}) \, n(\vec{r})$$

$$U[n] = E_{\text{H}}[n] + \Delta U[n] \qquad E_{\text{H}}[n] = \frac{e^2}{2} \int d^3r \int d^3r' \, \frac{n(\vec{r}) n(\vec{r'})}{|\vec{r} - \vec{r'}|}$$

Kohn-Sham: map onto a non-interacting system

- Separate, in $T[n]$, the kinetic energy of N non-interacting electrons but not necessarily homogeneous $T_s[n]$

$$T[n] = T_s[n] + T_c[n]$$

- Add the term E_{XC} that describe quantum effects (exchange and correlation) and the difference between $T[n]$ and $T_s[n]$

$$E_{xc}[n] = T_c[n] + \Delta U[n]$$

The energy functional rewritten

$$E[n] = T[n] + E_{\text{ext}}[n] + U[n]$$

$$U[n] = E_{\text{H}}[n] + \Delta U[n]$$

$$T[n] = T_s[n] + T_c[n]$$

$$E_{\text{xc}}[n] = T_c[n] + \Delta U[n]$$

$$E_{\text{ext}}[n] = \int d^3r \, V_{\text{ext}}(\vec{r}) \, n(\vec{r})$$

$$E_{\text{H}}[n] = \frac{e^2}{2} \int d^3r \int d^3r' \, \frac{n(\vec{r}) n(\vec{r'})}{|\vec{r} - \vec{r'}|}$$

$$E[n] = T_s[n] + \int d^3r \, V_{\text{ext}}(\vec{r}) \, n(\vec{r}) + E_{\text{H}}[n] + E_{\text{xc}}[n]$$

The Kohn-Sham equations

- Regroup all "potential" terms into a single-particle effective potential

$$V_s(\vec{r}) = V_{ext}(\vec{r}) + e^2 \int d^3r' \frac{n(\vec{r'})}{|\vec{r} - \vec{r'}|} + V_{xc}(\vec{r};[n])$$

$$V_{xc}(\vec{r};[n]) = \delta E_{xc}[n]/\delta n(\vec{r})$$

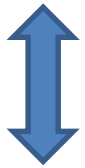
- Rewrite Schrödinger equation in terms of (solvable) <u>independent single-particle equations</u>

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_s(\vec{r})\right] \psi_j(\vec{r}) = \varepsilon_j \psi_j(\vec{r}) \qquad n_s(\vec{r}) = \sum_j f_j \mid \psi_j(\vec{r}) \mid^2$$

Ab initio molecular dynamics

- Solve quantum (equations, calculate ab initio enthalpies and forces (at T = 0 K)

$$E[n] = T_s[n] + \int d^3r\, V_{\mathrm{ext}}(\vec{r})\, n(\vec{r}) + E_{\mathrm{H}}[n] + E_{\mathrm{xc}}[n]$$



$$V(\mathbf{q}) = \frac{\langle \Psi_{\mathbf{q}} | H(\mathbf{q}) | \Psi_{\mathbf{q}} \rangle}{\langle \Psi_{\mathbf{q}} | \Psi_{\mathbf{q}} \rangle}$$

In the end, the *ab initio* energy and forces

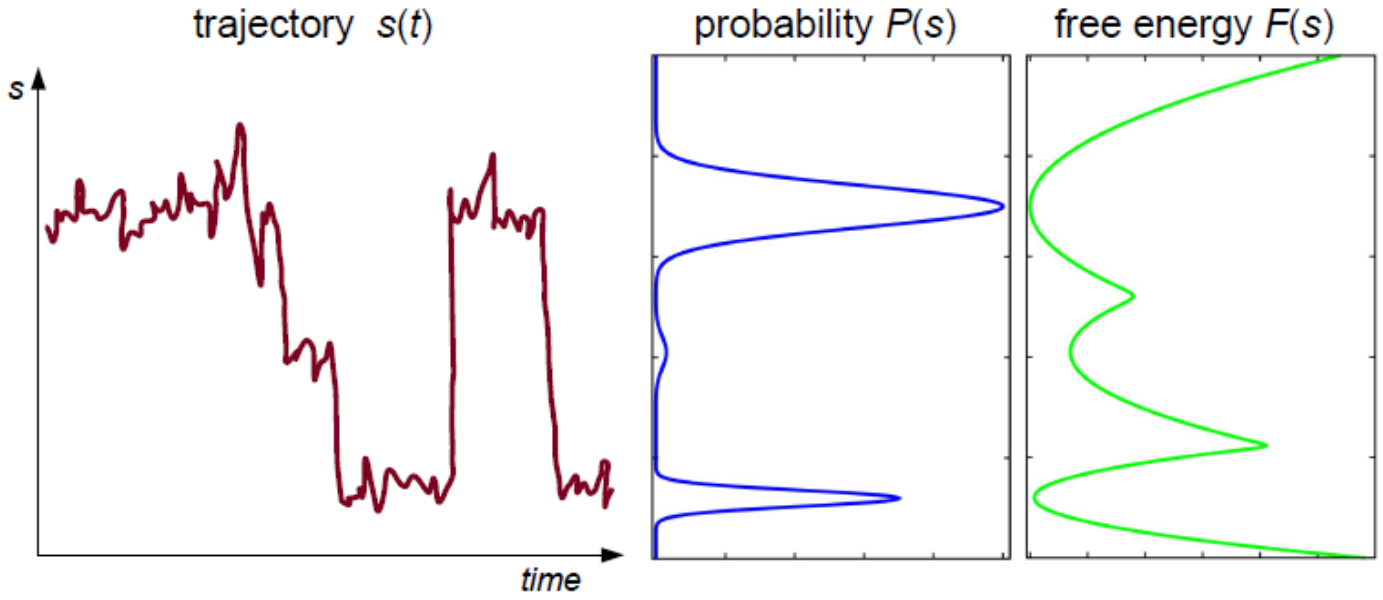
- Solve quantum (equations, calculate ab initio enthalpies and forces (at T = 0 K)

$$E[n] = T_s[n] + \int d^3r\, V_{\text{ext}}(\vec{r})\, n(\vec{r}) + E_{\text{H}}[n] + E_{\text{xc}}[n]$$

- Finite temperature: move atoms, explore (chemical) phase space

$$\mathbf{f}_i = m\,\ddot{\mathbf{r}}_i \qquad \mathbf{f}_i = -\frac{\partial U(\mathbf{r}^N)}{\partial \mathbf{r}_i} = -\vec{\nabla}_{\mathbf{r}_i} U(\mathbf{r}^N)$$

Connection AIMD – Statistical mechanics



from probabilities (histograms) we get free energies:

$$P(s) = \lim_{t\to\infty} \frac{1}{t} \int_0^t dt\ \delta(s - s(x(t))) \qquad F(s) = -\frac{1}{\beta} \log P(s)$$

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- What: "generalized" structural transformations in condensed matter physics and chemistry
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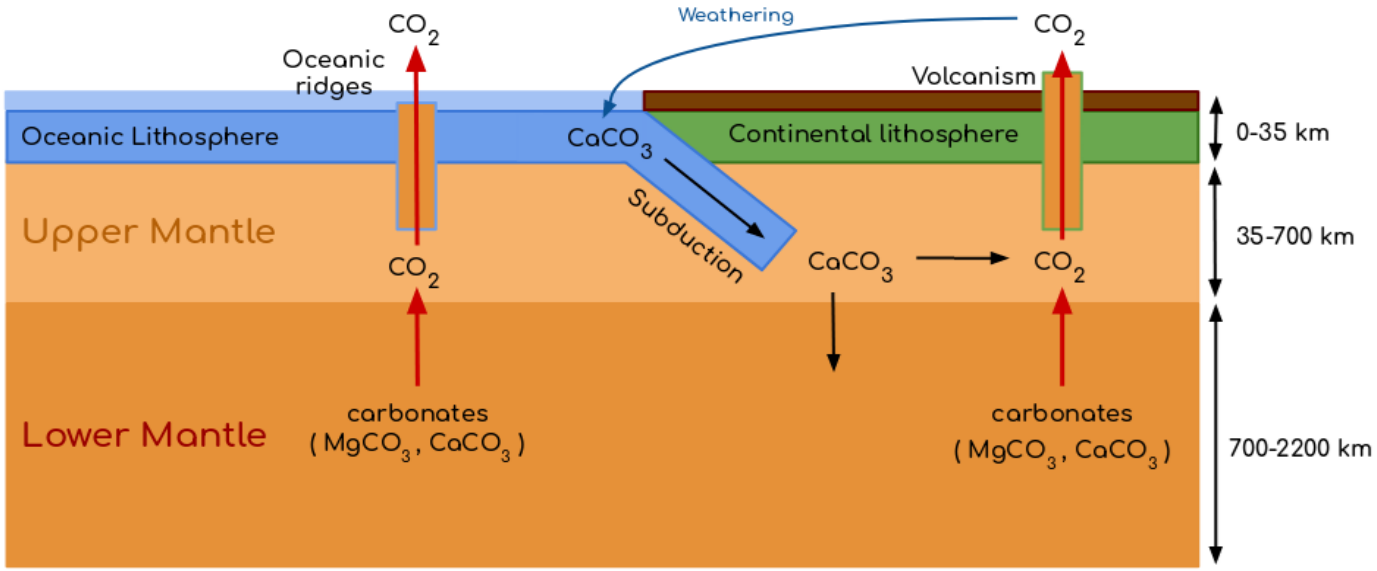
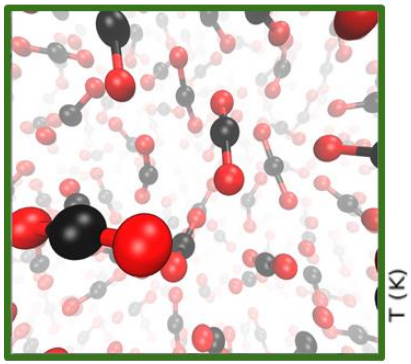
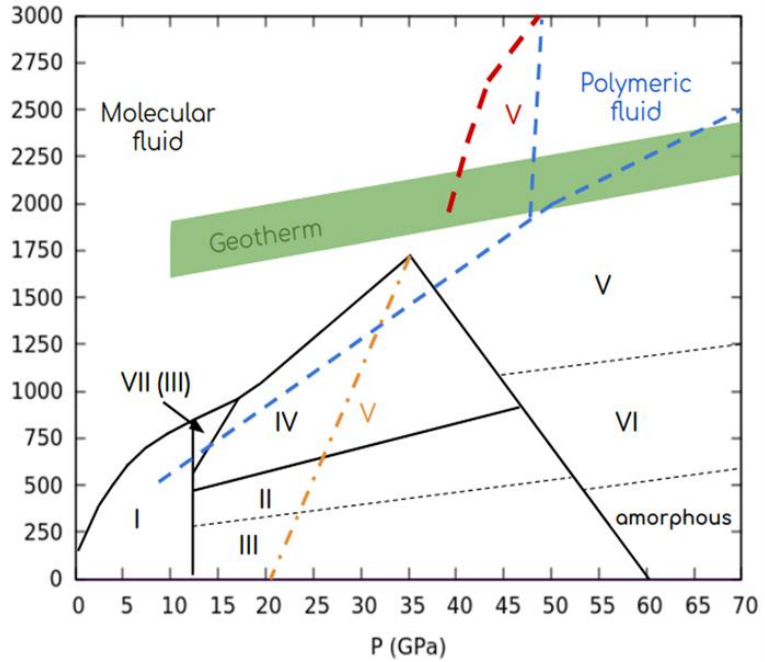
Geological fluid CO_2 (thesis of M. Moog)

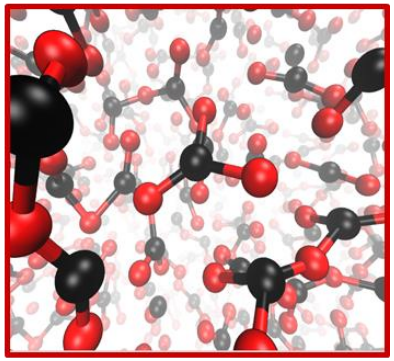


- An essential component of geological physics and chemistry
- Subject to many potential "transformations", both intrinsic and extrinsic

Pressure/temperature phase diagram of CO_2

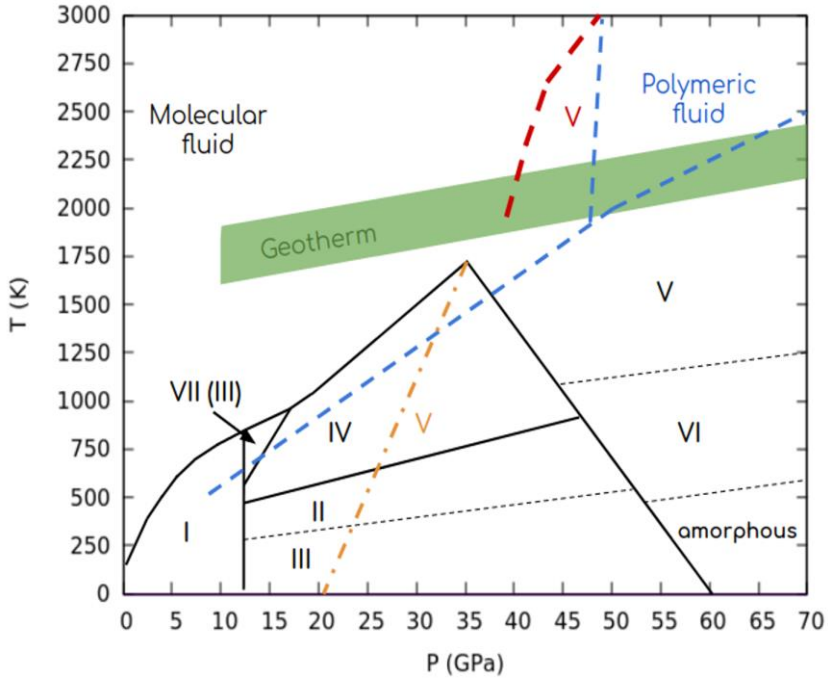






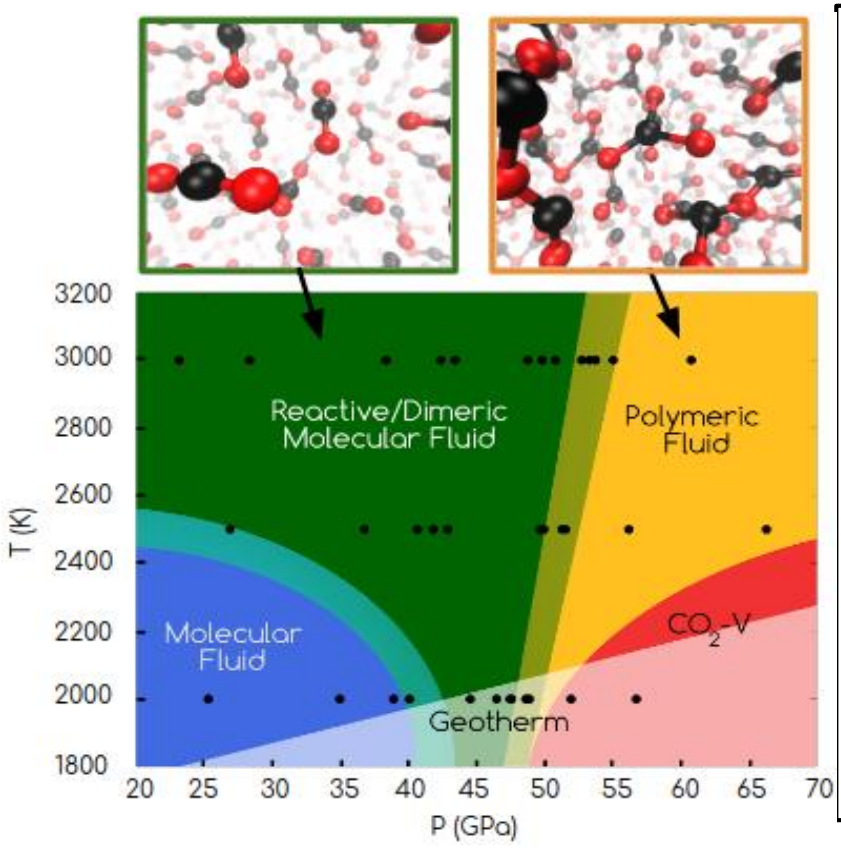
- Two major regimes: molecular (up to 40 Gpa) and polymeric (beyond)
- Many crystalline phases, and several possible disordered (liquid, amorphous) forms

CO_2 phase diagram exploration by ab initio molecular dynamics



- 45 different P/T points (3 temperatures, 15 pressures)
- 100-ps long trajectories, ~5ns trajectories in total
- 32 CO_2 molecules

Ab initio phase diagram of CO_2



Four different regimes:

- **"Standard" molecular liquid:** composed of individual CO_2 molecules
- **Reactive/Dimeric molecular fluid:** formation of dimers (and trimers), exchange of O between molecules
- **Polymeric fluid:** Extremely dynamic fluid with a complex chain network in perpetual evolution
- **Glassy system or CO_2-V:** CO2-V likely most stable in "real" experimental conditions.

M. Moog, F. Pietrucci, AMS, *under evaluation* (2020)

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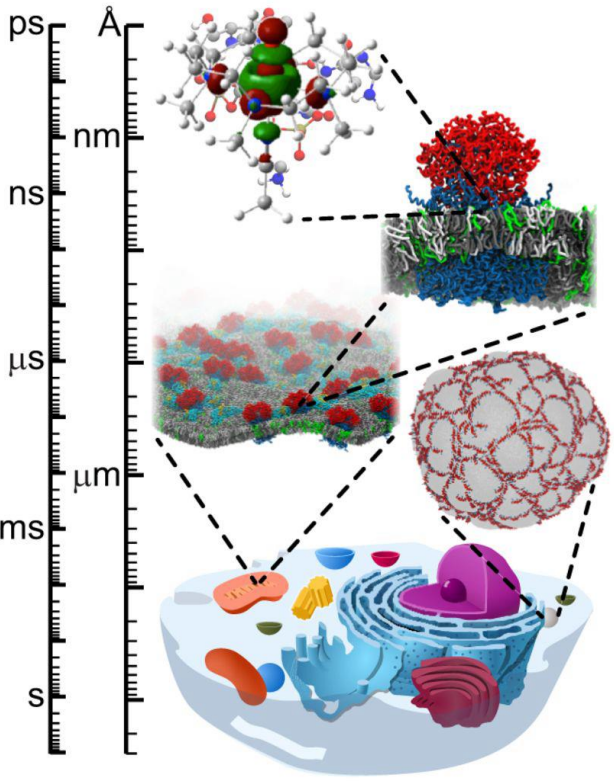
A general overview of our scientific interests (with Fabio Pietrucci)



Quantum
- atoms, electrons and electron clouds included
- explicit solvent
- quantum mechanics

All-atom
- all or most atoms present
- explicit solvent
- molecular dynamics

Coarse-grained
- beads comprising a few atoms
- explicit or implicit solvent
- molecular dynamics

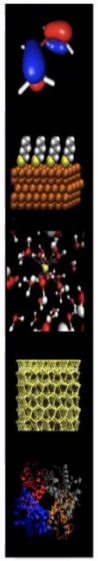
Supra-coarse-grained
- interaction sites comprising many atoms, protein parts or proteins
- implicit solvent
- stochastic dynamics

Continuum
- materials as a continuous mass
- implicit solvent
- continuum mechanics

Accuracy

Efficiency

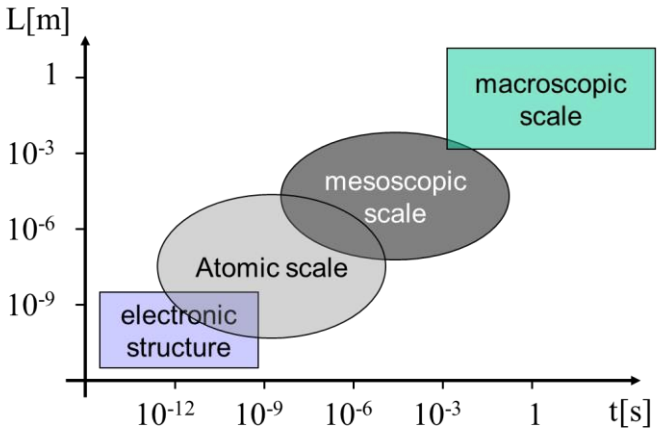
Method	Atoms	Simulation Time
CI, CC, MP2, MP4, ...	10 - 100	0
Density Functional Theory	100 - 1000	100 ps
Semiempirical Methods Tight Binding	1000 - 10 000	1 ns
„Reactive Potentials" EAM, Tersoff, ...	1000 - 100 000	10 ns
Classical Force Fields (LJ, harmonic, Coulomb)	1 000 000	1 ms



- Challenge n.2 : replace costly ab initio simulations by machine-learning-based ones

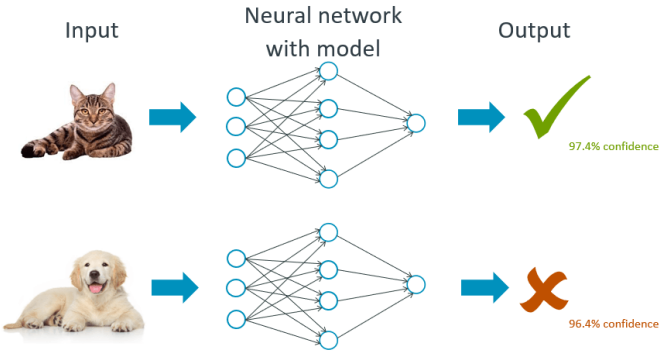
General principles of machine-learning approaches in *ab initio* computational materials science

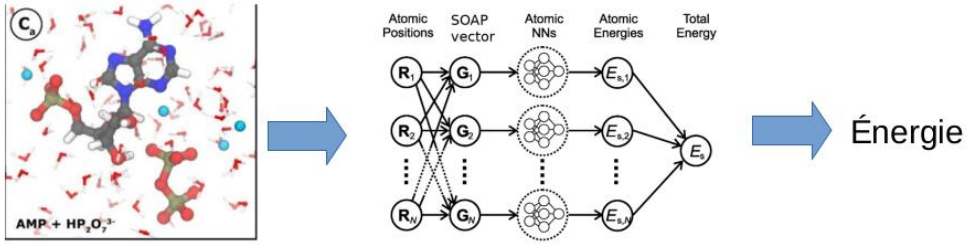
- *Ab initio* ("electronic structure") calculations are generally very expensive
  - DFT~ N^3
  - Quantum Monte Carlo ~ N^4
  - Adv quantum chem ~ N^{6-7}
- *Ab initio* trajectories ~ *ns* timescale at the best
- CO_2 trajectories: ~2.5 million supercomputer hours ~ 6-8 months of human time at best
- Even using metadynamics or other enhanced sampling methods, this is a **major bottleneck**

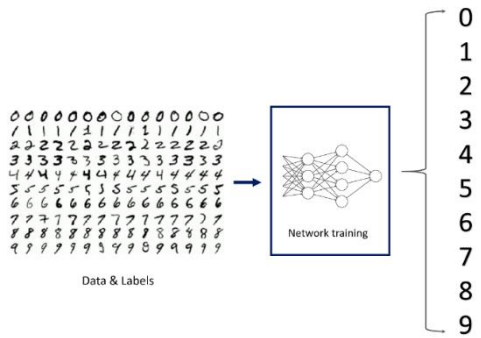


General principles of machine-learning approaches in *ab initio* computational materials science

- Neural networks can "learn", by training, to recognize a cat from a dog, or handwritten numbers
- Can we train neural networks to "recognize" atomic configurations, and univocally associate to them physical quantities (energy, forces, etc…)?
- Can we exploit our long *ab initio* trajectories?



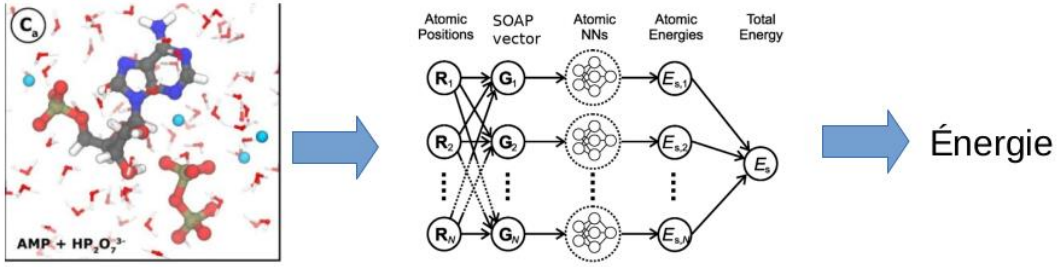




PhD thesis of Julien Heu

General principles of machine-learning approaches in *ab initio* computational materials science

- "Fitting" quantum-based physical interactions is not new (it is what "classical model potentials" do)
- Founder of the method: Jörg Behler (Univ Göttingen)
- Building a NNP can be done:
  - without any a priori knowledge/choice of the mathematical form of the potential
  - with a "local" perspective: $E_{tot} = \sum_i^{N_{atoms}} E_i$

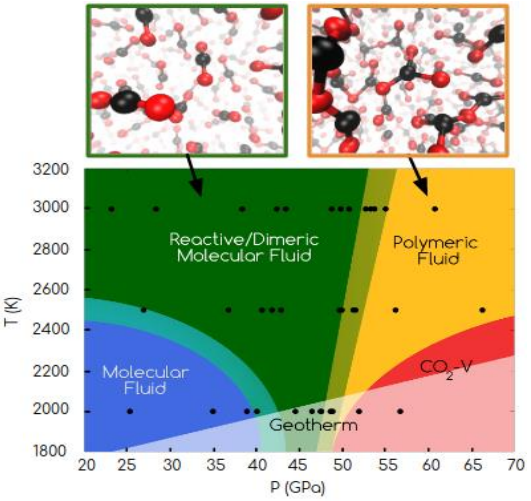


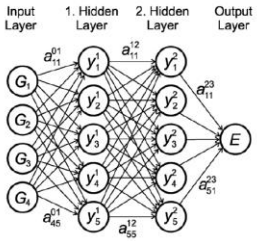
General principles of machine-learning approaches in *ab initio* computational materials science

- We use structural descriptors with rotational and translational symmetries: Smooth Overlap of Atomic Positions (SOAP)

- Local approach, *i.e.* for a single CO_2 molecule:

- Differences with standard fitting techniques
  - Hierarchy and non-linearities
  - Stochastic gradient descents





$$y_m^n = f_m^n(x_m^n) = f_m^n\left(b_m^n + \sum_{i=1}^{N_{n-1}} y_i^{n-1} a_{im}^{n-1,n}\right). \qquad (3)$$

$$E = f_1^3\left(b_1^3 + \sum_{l=1}^{5} a_{l1}^{23} \cdot f_l^2\left(b_l^2 + \sum_{k=1}^{5} a_{kl}^{12} \cdot f_k^1\left(b_k^1 + \sum_{j=1}^{4} a_{jk}^{01} \cdot G_j\right)\right)\right).$$

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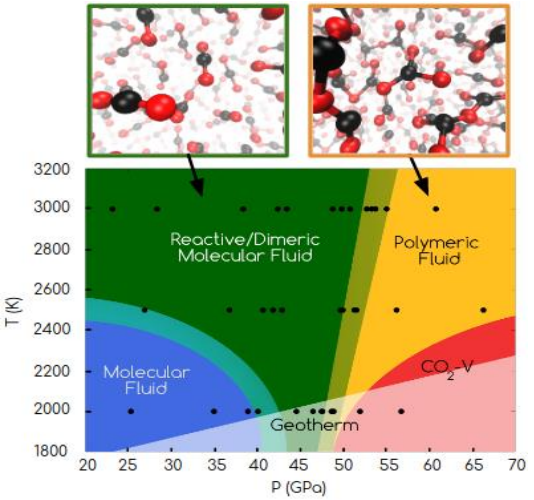
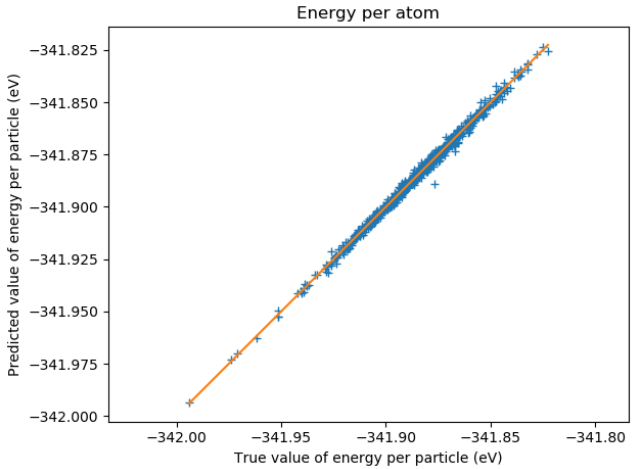
- Evaluating the quality





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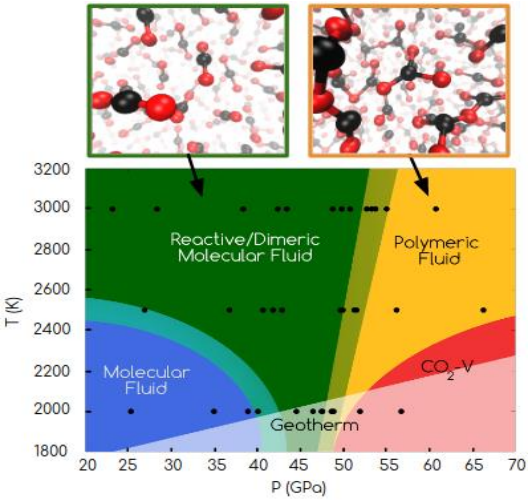

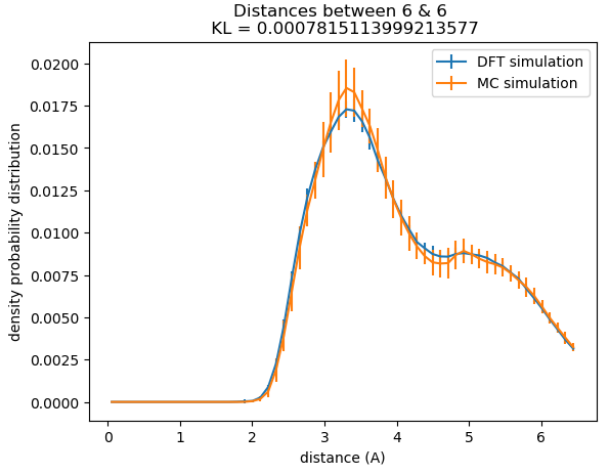

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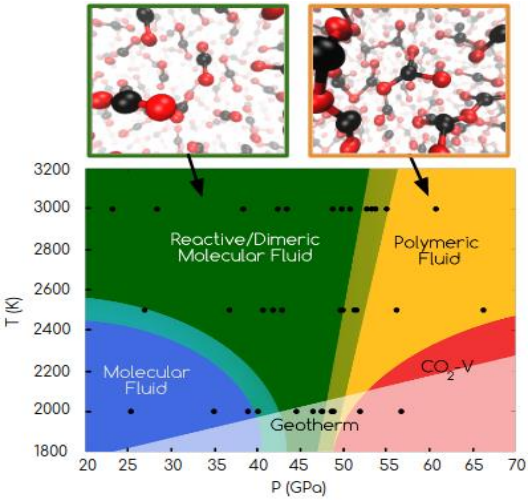

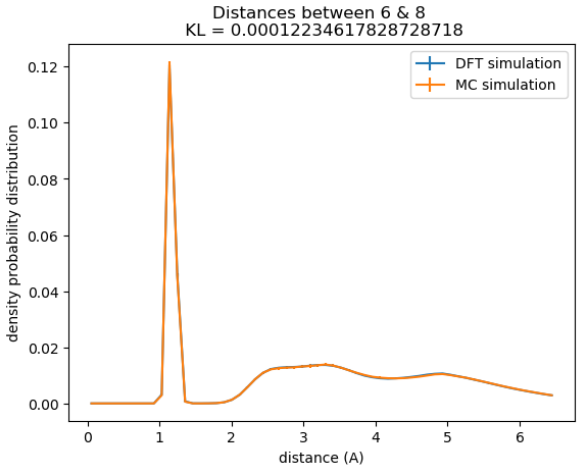

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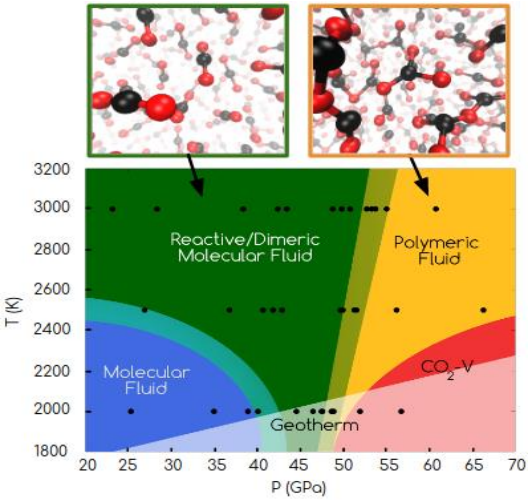

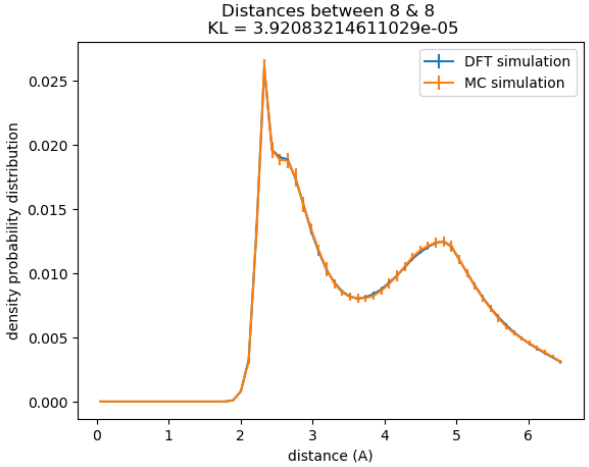

Conclusions

- What: "generalized" structural transformations in condensed matter physics and chemistry
  - Phase transitions (under pressure)
  - Nucleation from the liquid phase
  - Chemical reactions in solutions
  - Protein structure-function relations
- How: computer simulations of *ab initio* (= quantum) molecular dynamics
- One emblematic case: CO_2 at "geological" conditions
- Bottleneck: efficient sampling of 3N-dimensional configurational space
- Challenge n.1 : find "good" collective variables to describe/project the manifold onto a few relevant dimensions
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MAESTRO

Institut des sciences du calcul et des données
SORBONNE UNIVERSITÉ

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