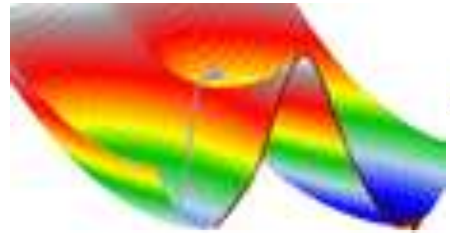
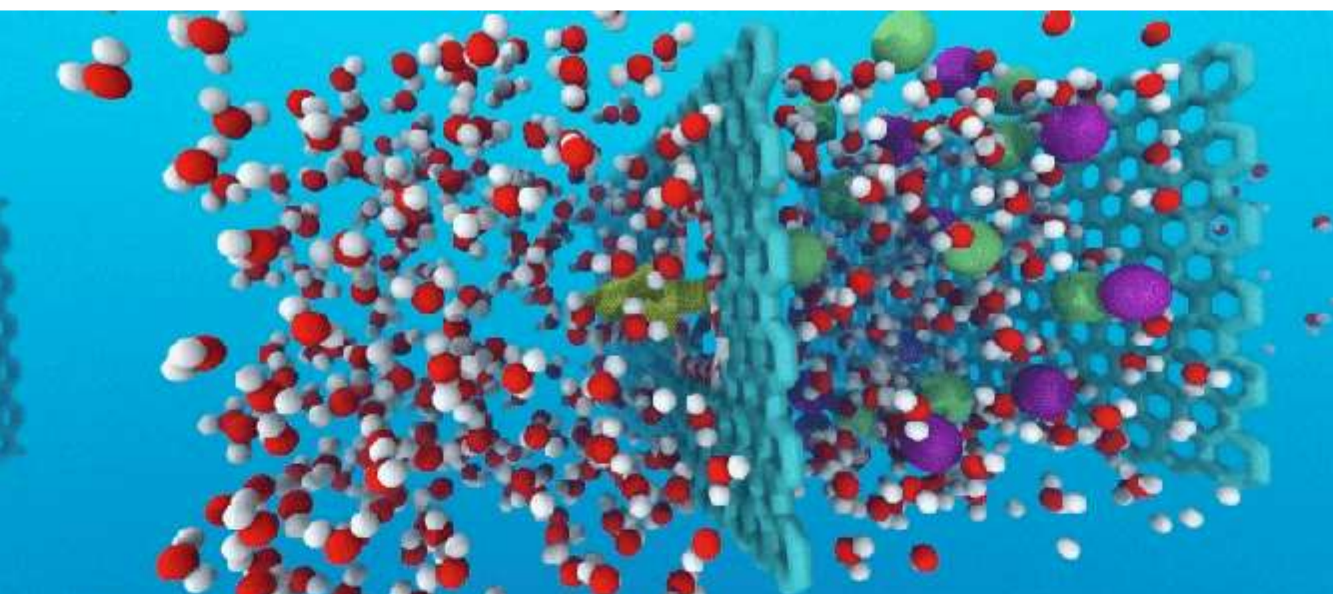
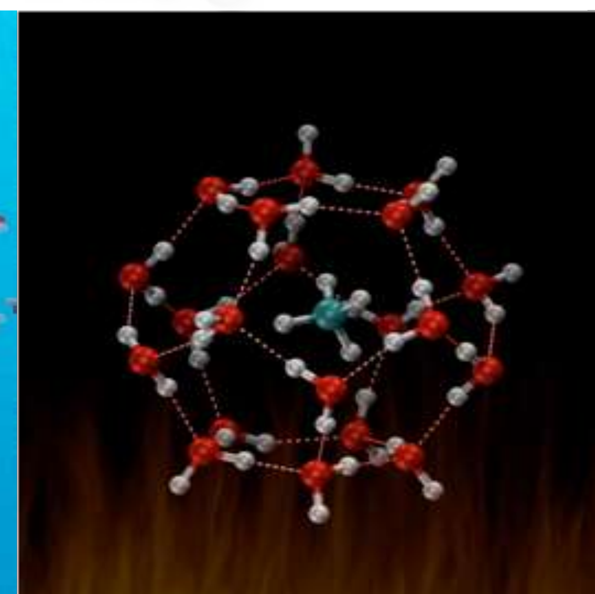


Computational Materials Science, Physics and Chemistry

M2-Science des Matériaux et Nano-Objets/NANOMAT
M2-Chimie Théorique

A. Marco Saitta





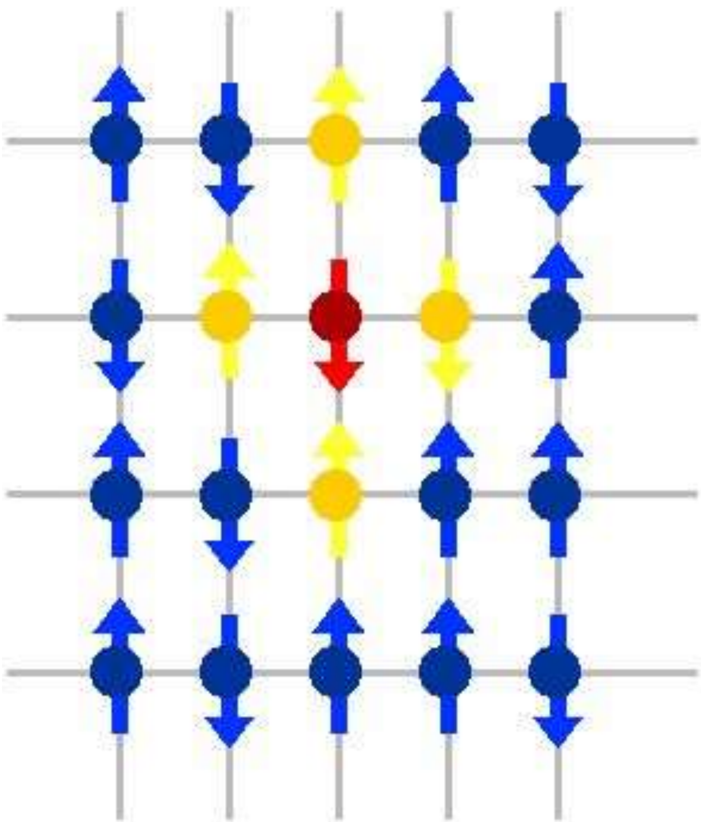
Computational Physics: why?

- The vast majority of physics problems has no analytical solution
- Solvers are not necessarily capable of solving complex problems
- Simulations allow to explore fictitious worlds, impacting from meteorology to stock exchange

Simulations in Statistical Mechanics

- Example: Ising model

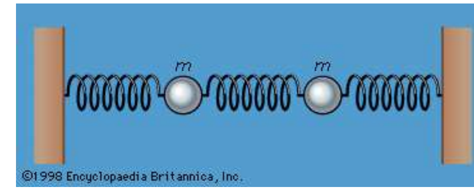
$$H(\sigma) = -\sum_{<i\ j>} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j$$

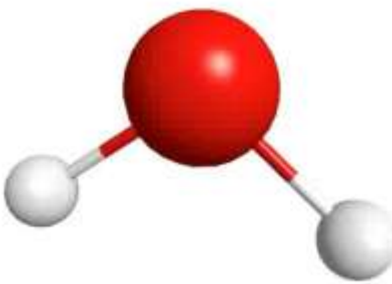


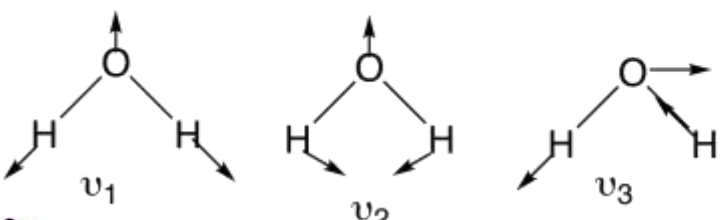
$$H(\sigma) = -J\sum_{<i\ j>} \sigma_i\sigma_j$$

Atomic-level interactions

- Example: Molecular vibrations in CO_2, H_2O
  - Coupled oscillators: eigenvalue problem

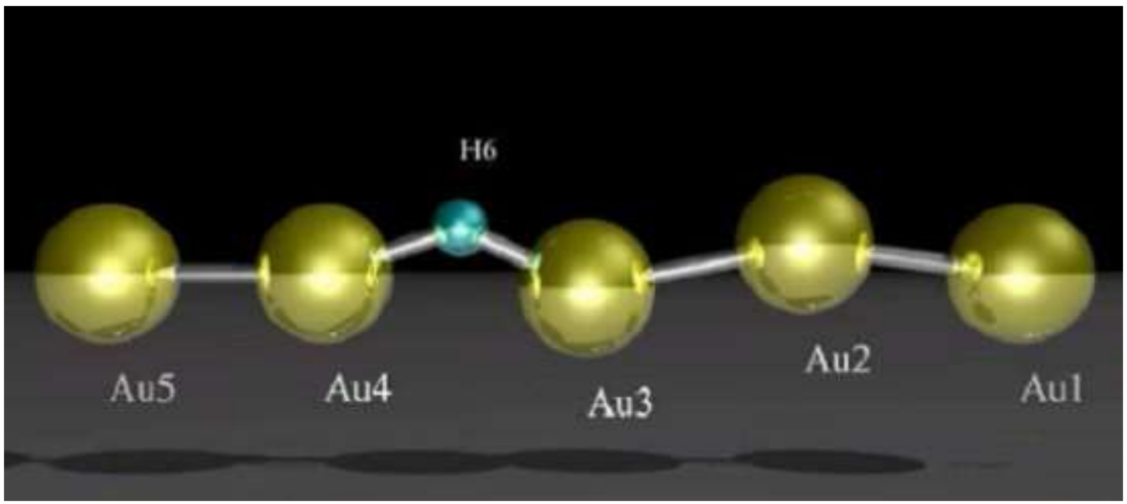






Molecular vibrations

- Polyatomic chain? Impurities?



Numerical simulations!!

$$A = \begin{bmatrix} a_{11} & a_{21} & 0 & . & . & . & 0 \\ a_{21} & a_{22} & a_{32} & 0 & & & . \\ 0 & a_{32} & a_{33} & a_{43} & 0 & & . \\ . & 0 & a_{43} & a_{44} & . & . & . \\ . & & 0 & . & . & . \; . & \\ . & & & . & . & . \; . & . \\ & & & & . & . \; . & . \\ 0 & . & . & . & & . \; . & a_{nn} \end{bmatrix}$$

Research in physics and in condensed matter physics/materials science

- General Physics 12 %
- Gravitation and Astrophysics 5 %
- Elementary Particles and Fields 5 %
- Nuclear Physics 2 %
- Atomic, Molecular, and Optical Physics 6 %
- Nonlinear/Fluid Dynamics 10 %
- Plasma and Beam Physics 4 %
- Condensed Matter: Structure, etc.
- Condensed Matter: Electronic Properties, etc.
- Soft Matter, Biological, Interdisciplinary Physics

Physical Review Letters
moving physics forward

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General Physics	12 %
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Nuclear Physics	2 %
Atomic, Molecular, and Optical Physics	6 %
Nonlinear/Fluid Dynamics	10 %
Plasma and Beam Physics	4 %
Condensed Matter: Structure, etc.	**14 %**
Condensed Matter: Electronic Properties, etc.	**31 %**
Soft Matter, Biological, Interdisciplinary Physics	**11 %**

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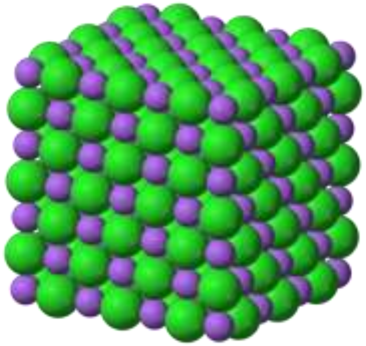
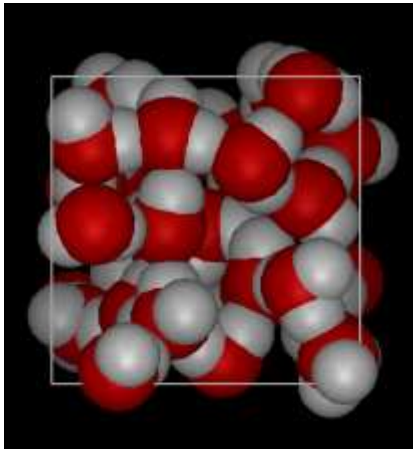
Computational Condensed Matter Physics and Chemistry

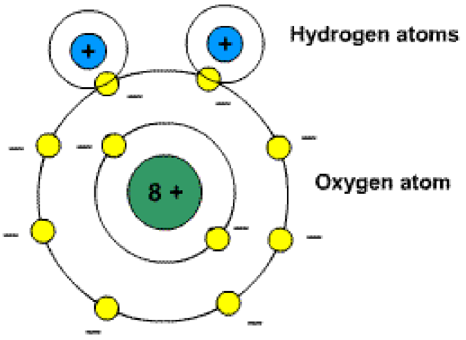
- Condensed matter : many particles



- Atomic/molecular interactions



- Electrons



Super-brief history of computer simulations (in condensed matter)

- 99 BC – 55 BC: **Titus Lucrecius**

« The atoms are eternal and always moving. Everything comes into existence simply because of the random movement of atoms, which, given enough time, will form and reform, constantly experimenting with different configurations of matter from which will eventually emerge everything we know... »

Super-brief history of computer simulations (in condensed matter)

- 99 BC – 55 BC: **Titus Lucrecius**

- 1929: **PAM Dirac**

« The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations that are much too complicated to be soluble. »

Super-brief history of computer simulations (in condensed matter)

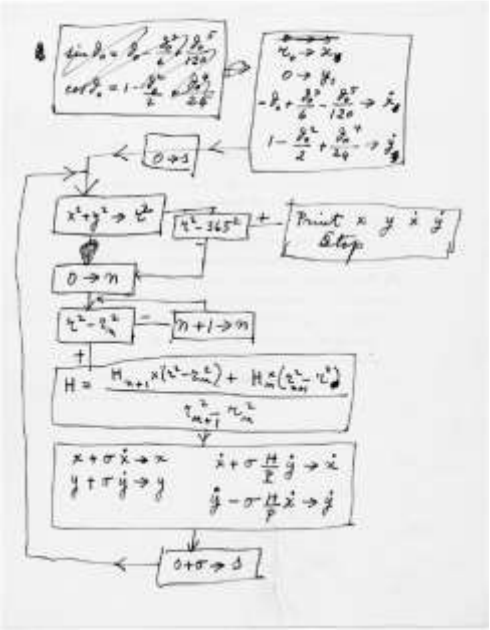
- 99 BC – 55 BC: **Titus Lucrecius**

- 1929: **PAM Dirac**

  « The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations that are much too complicated to be soluble. **It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to explanation of the main features of complex atomic systems without too much computation. »**

Super-brief history of computer simulations (in condensed matter)

- 99 BC – 55 BC: **Titus Lucrecius**
- 1929: **PAM Dirac**
- **Enrico Fermi**



What happened before (or without) computers ?

- Theories but only few exact and most of them approximate

- Bernal did mechanical simulations of large assemblies of macroscopic spheres (e.g. rubber balls and ball bearings)

Extract from J.D. Bernal, The Bakerian Lecture, 1962:

The rest of this lecture will be an attempt to construct on these minimal hypotheses a rational and verifiable image of liquid structures. I began, rather naïvely, by attempting to build models just to see what a structure satisfying these conditions would look like. I took a number of rubber balls and stuck them together with rods of a selection of different relative lengths ranging from 2·75 to 4 in. I tried to do this in the first place as casually as possible, working in my own office, being interrupted every five minutes or so and not remembering what I had done before the interruption.

What happened before (or without) computers ?

- **Bernal did mechanical simulations of large assemblies of macroscopic spheres (*e.g.* rubber balls and ball bearings)**

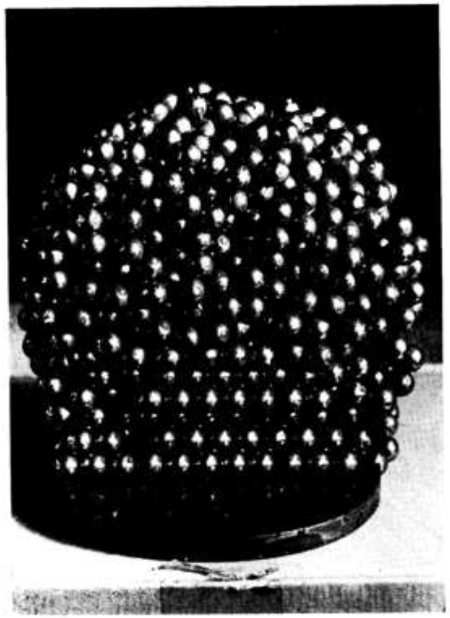


FIGURE 16. Ball-bearing assembly showing transition from random close-packing t regular crystalline array induced by inserting a flat plate.

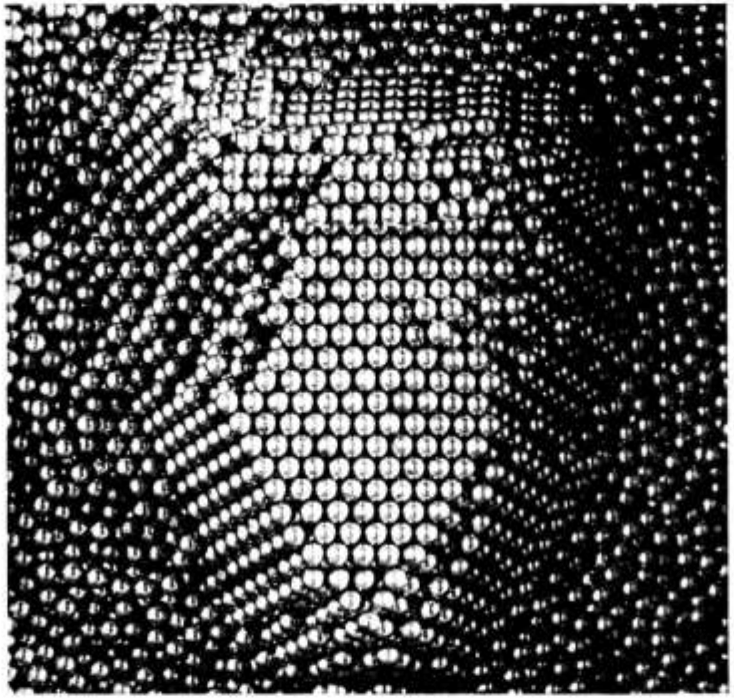


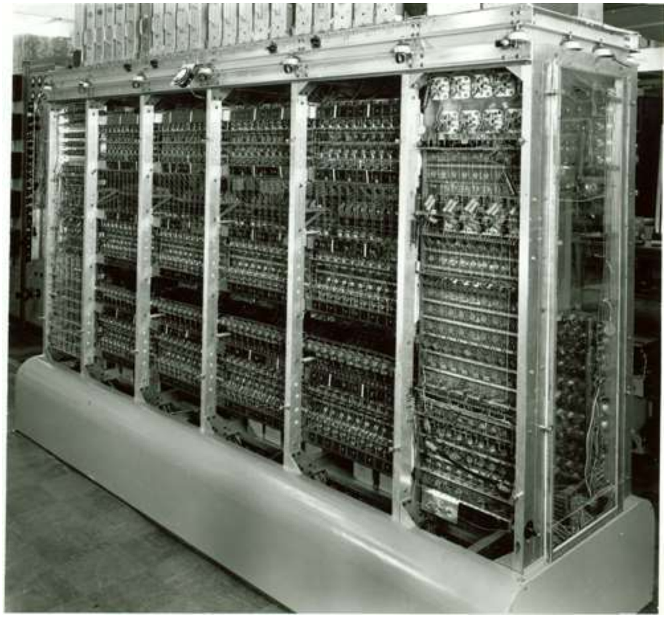
FIGURE 14. Face-centred cubic 'crystal' surrounded by 'liquid' caused by shearing ball-bearing mass. 111 face is shown at the top surface.

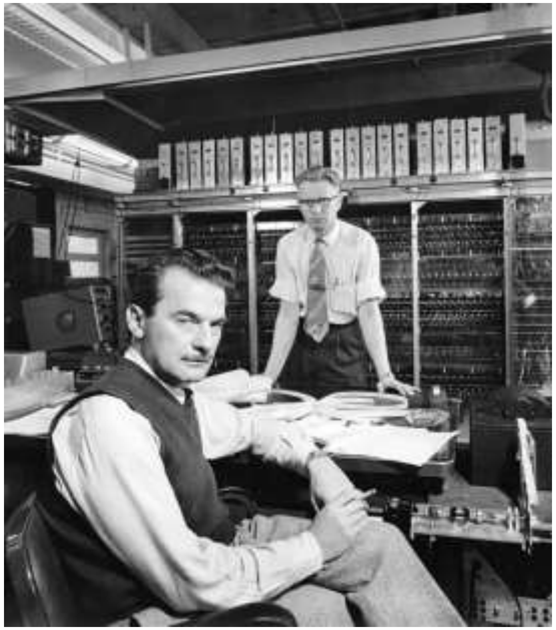
Super-brief history of computer simulations (in condensed matter)

- 1939-1945 (World War II): **Nuclear Weapon Development** and **Code Breaking**

- 1950s: Electronic **computers** available for **nonmilitary use**

- 1952: Los Alamos **MANIAC** became operational (under the direction of N. **Metropolis**)





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- 1950s: Electronic **computers** available for **nonmilitary use**

- 1952: Los Alamos **MANIAC** became operational (under the direction of N. **Metropolis**)

- 1953: Milestone publication of **Metropolis** on **Monte Carlo (MC)** simulations

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

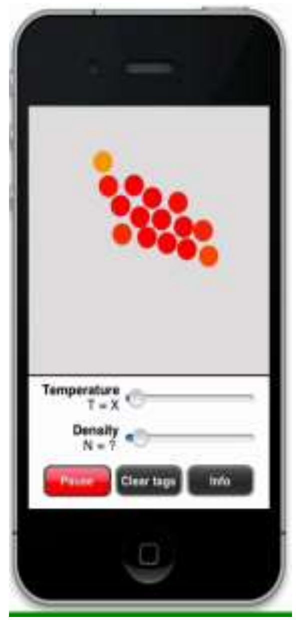
Equation of State Calculations by Fast Computing Machines

Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, and Augusta H. Teller,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

Edward Teller,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

Super-brief history of computer simulations (in condensed matter)



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NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

Super-brief history of computer simulations (in condensed matter)

- 1957: First **Molecular Dynamics** (MD) simulation of **Hard Spheres**

- 1957: Meeting in New Jersey (USA) with 15 scientists (2 Nobel laureates) – Can **hard spheres** form a **stable crystal**?

- Half the audience answered **YES**

- Work of Alder and Wainwright proved the predictive power of computers

Phase Transition for a Hard Sphere System

B. J. Alder and T. E. Wainwright
University of California Radiation Laboratory, Livermore, California
(Received August 12, 1957)

A CALCULATION of molecular dynamic motion has been designed principally to study the relaxations accompanying various nonequilibrium phenomena. The method consists of solving exactly (to the number of significant figures carried) the simultaneous classical equations of motion of several hundred particles by means of fast electronic computors. Some of the details as they relate to hard spheres and to particles having square well potentials of attraction have been described.[1,2] The method has been used also to calculate equilibrium properties, particularly the equation of state of hard spheres where differences with previous Monte Carlo[3] results appeared.

The calculation treats a system of particles in a rectangular box with periodic boundary conditions.[4]

Super-brief history of computer simulations (in condensed matter)

- **1959: First MD simulation of real material by Vineyard group**

PHYSICAL REVIEW VOLUME 120, NUMBER 4 NOVEMBER 15, 1960

Dynamics of Radiation Damage*

J. B. Gibson, A. N. Goland,† M. Milgram, and G. H. Vineyard
Brookhaven National Laboratory, Upton, New York

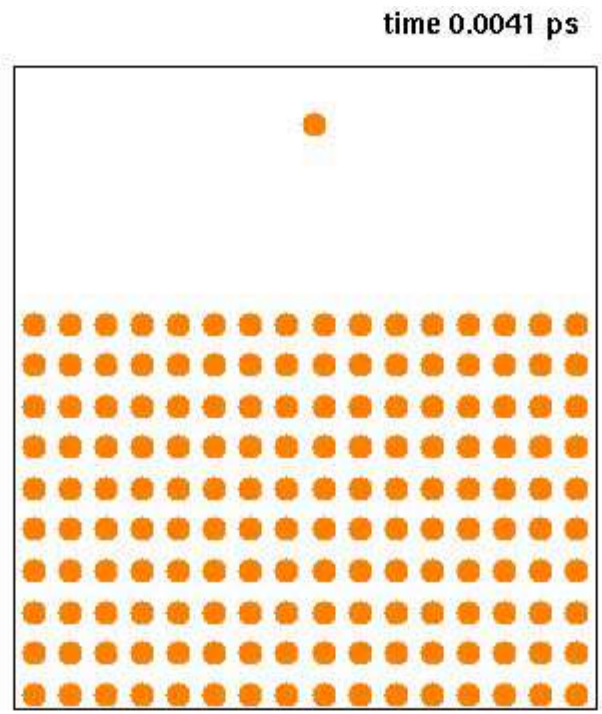
(Received July 14, 1960)

Radiation damage events at low and moderate energies (up to 400 ev) are studied by machine calculations in a model representing copper. Orbits of knock-on atoms are found and the resulting damaged configurations are observed to consist of interstitials and vacancies. Thresholds for producing permanently displaced atoms (i.e., interstitials) are about 25 ev in the ⟨100⟩ direction, 25 to 30 ev in the ⟨110⟩ direction, and around 85 ev in the ⟨111⟩ direction. Collision chains in the ⟨100⟩ and ⟨110⟩ directions are prominent; at low energies the chains focus, at higher energies they defocus. Above threshold, the chains transport matter, as well as energy, and produce an interstitial at a distance. The range of ⟨110⟩ chains has been studied in detail. Localized vibrational modes associated with interstitials, agitations qualitatively like thermal spikes, ring annealing processes, and a higher energy process somewhat like a displacement spike have been observed. Replacements have been found to be very numerous.

The configurations of various static defects have also been studied in this model. The interstitial is found to reside in a "split" configuration, sharing a lattice site with another atom. The crowdion is found not to be stable, and Frenkel pairs are stable only beyond minimum separations, which are found to be very much dependent on orientation.

Super-brief history of computer simulations (in condensed matter)

- 1959: First MD simulation of real material by Vineyard group



...and now?

The Nobel Prize in Chemistry 2013

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Chemistry for 2013 to

Martin Karplus
Université de Strasbourg, France and Harvard University, Cambridge, MA, USA

Michael Levitt
Stanford University School of Medicine, Stanford, CA, USA

Arieh Warshel
University of Southern California, Los Angeles, CA, USA

"for the development of multiscale models for complex chemical systems"

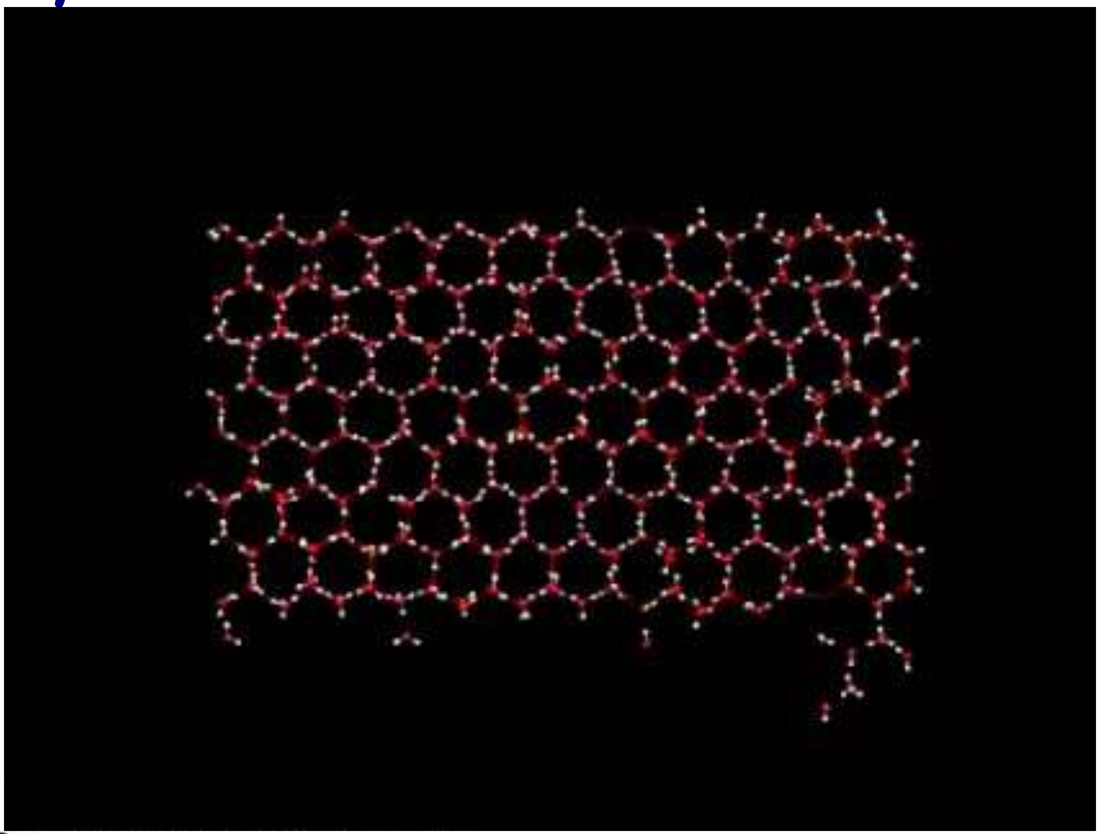
The computer — your Virgil in the world of atoms

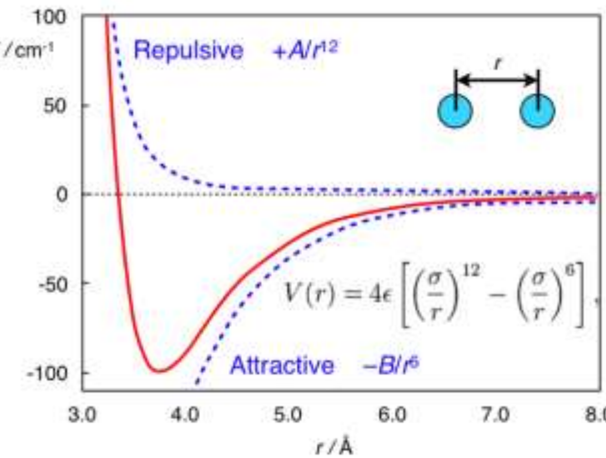
Chemists used to create models of molecules using plastic balls and sticks. Today, the modelling is carried out in computers. In the 1970s, **Martin Karplus, Michael Levitt** and **Arieh Warshel** laid the foundation for the powerful programs that are used to understand and predict chemical processes. Computer models mirroring real life have become crucial for most advances made in chemistry today.

This year's Nobel Laureates in chemistry took the best from both worlds and devised methods that use both classical and quantum physics. For instance, in simulations of how a drug couples to its target protein in the body, the computer performs quantum theoretical calculations on those atoms in the target protein that interact with the drug. The rest of the large protein is simulated using less demanding classical physics.

Behavior of condensed matter

- **Classical methods: molecular dynamics**



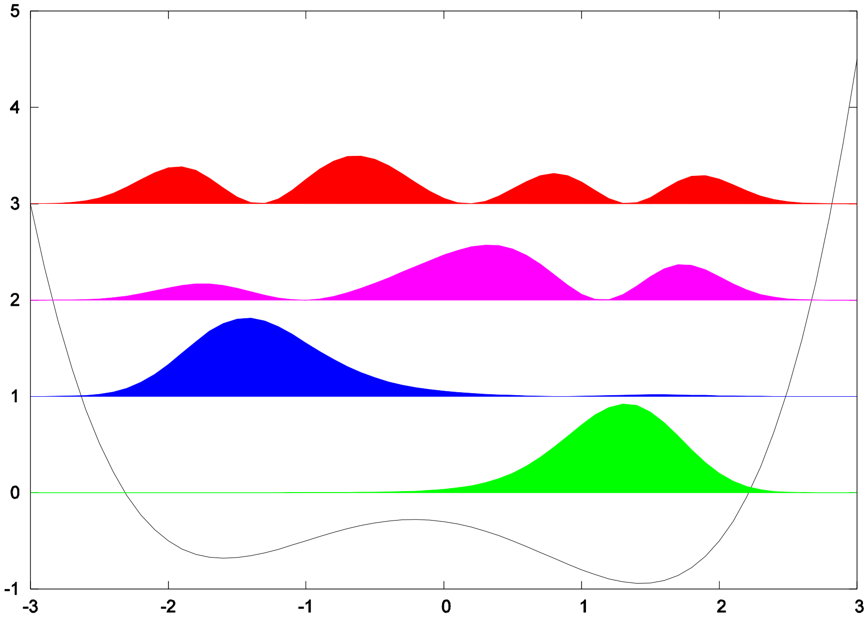


$$\mathbf{f}_i = m\,\ddot{\mathbf{r}}_i$$

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

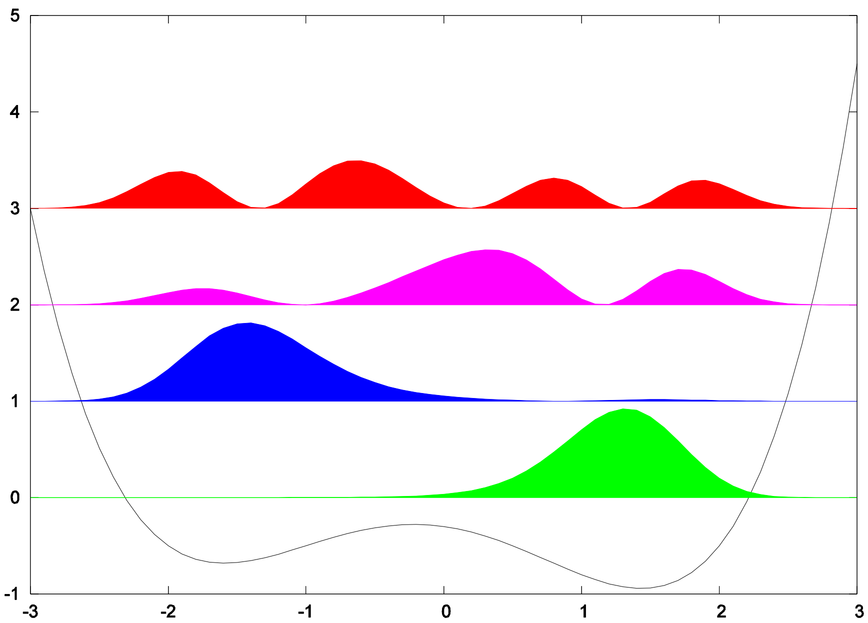
Quantum mechanics

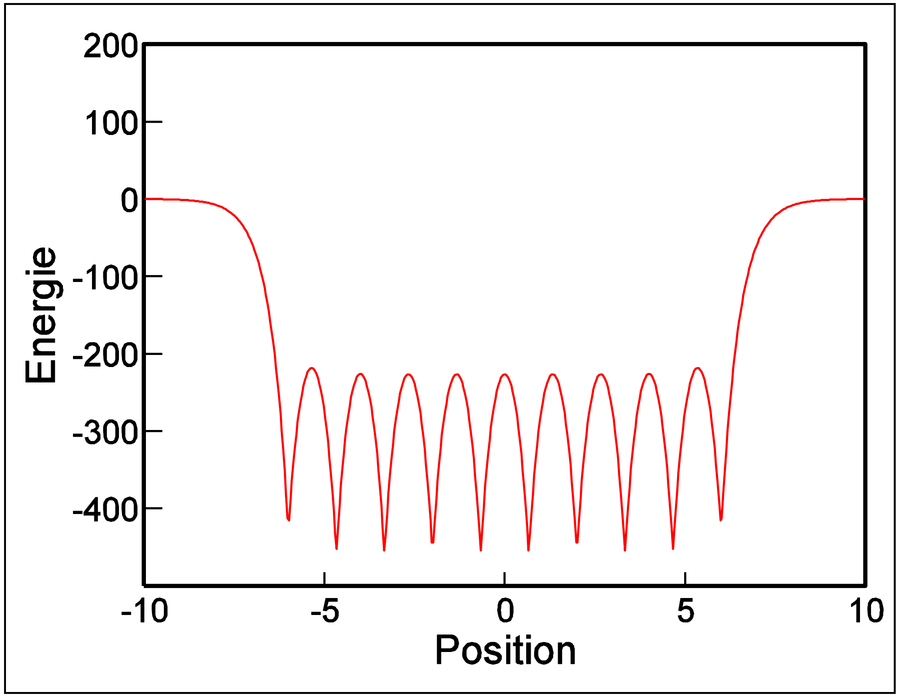
- Double-well potential, 1 particle, 1D: easy numerical solution (diagonalization of a 10^2x10^2 matrix)



Quantum mechanics

- Multiple-well (atomic-chain) potential, 1 particle, 1D: easy numerical solution (diagonalization of a $10^2 \times 10^2$ matrix)





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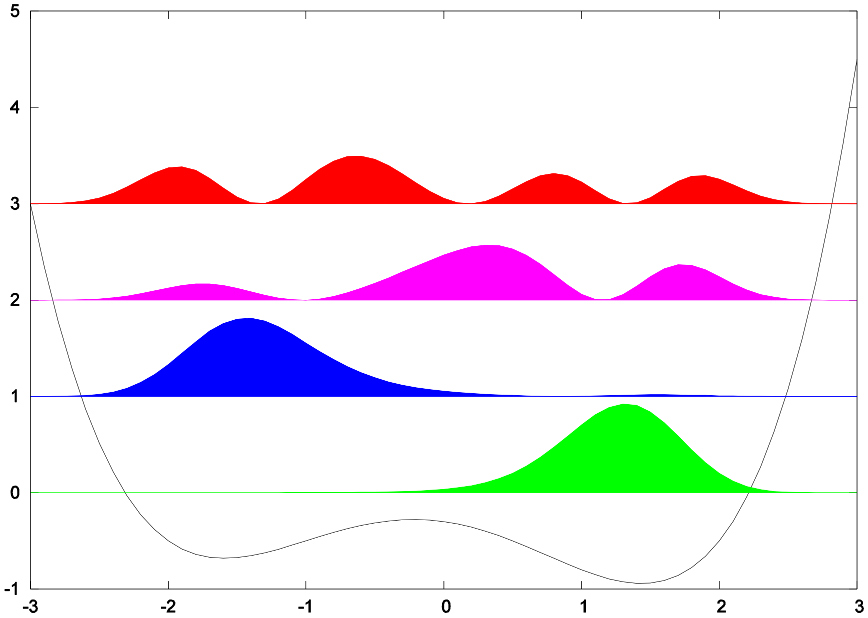
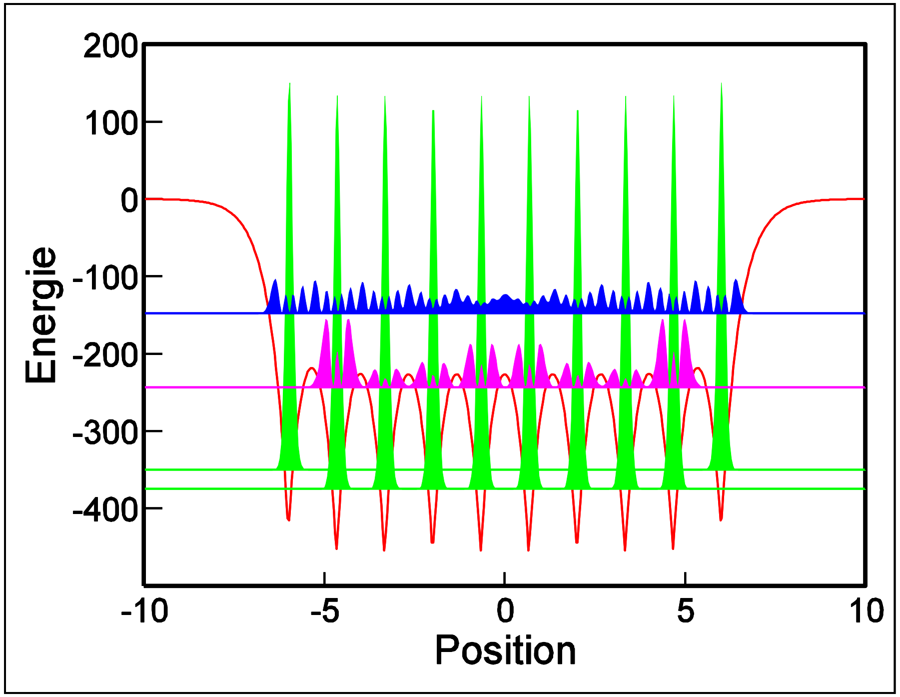




Quantum mechanics

- Multiple-well (atomic-chain) potential, 1 particle, 1D: easy numerical solution (diagonalization of a 10^2x10^2 matrix)
- Multiple-well (solid-like) potential, 1 particle, 3D: diagonalization of a 10^6x10^6 matrix…
- Atome d'hélium, 2 particles, 3D: diagonalization of a 10^{12}x10^{12} matrix !!

Quantum mechanics in real systems

- Solution? Algorithms, but especially theory!!
- Hartree, Hartree-Fock, quantum chemistry
- Density-Functional Theory (DFT)

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

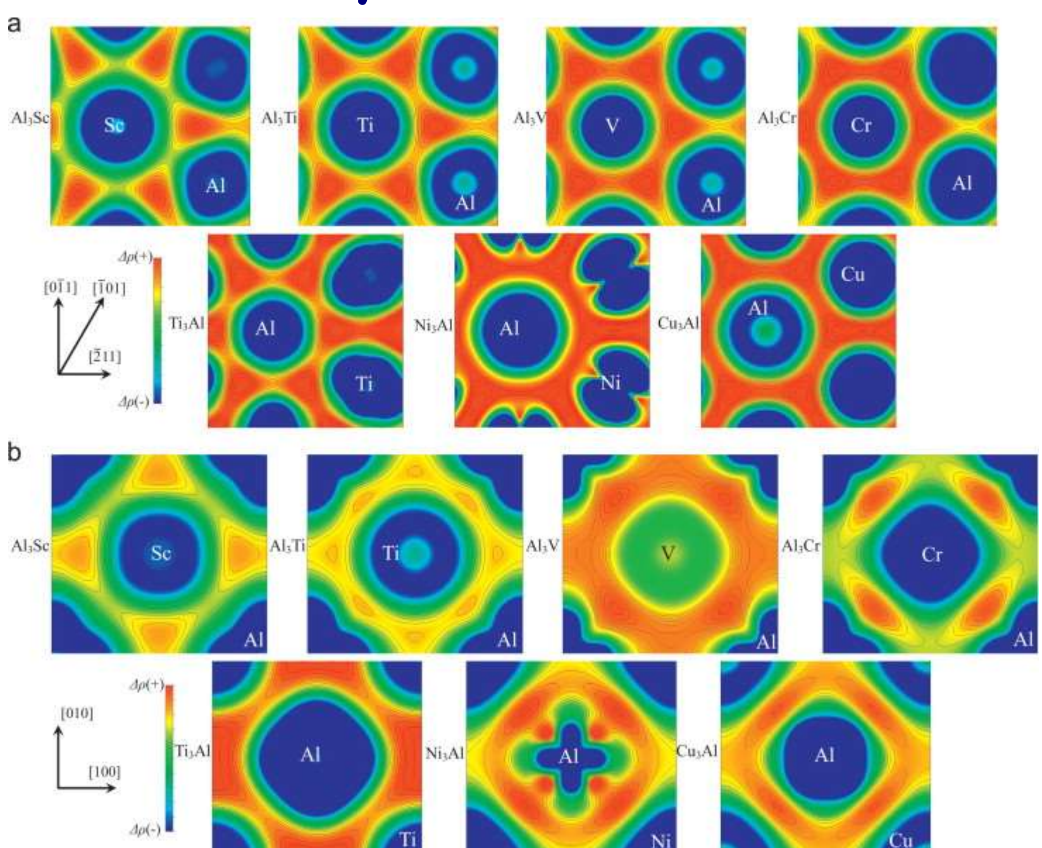
$$\left[-\frac{\hbar^2 \nabla_2}{2m} + V_{\rm ext}(\vec{r}) + e^2 \int d^3r' \, \frac{n(\vec{r'})}{|\vec{r} - \vec{r'}|} + V_{\rm xc}(\vec{r};[n])\right] \psi_j(\vec{r}) = \varepsilon_j \psi_j(\vec{r})$$

$$n(\vec{r}) = \sum_j f_j \, | \psi_j(\vec{r}) |^2$$

(Density Functional) Theory

- Electrons

  -> "exact" theory ! ~10^2 atoms, ~10 ps



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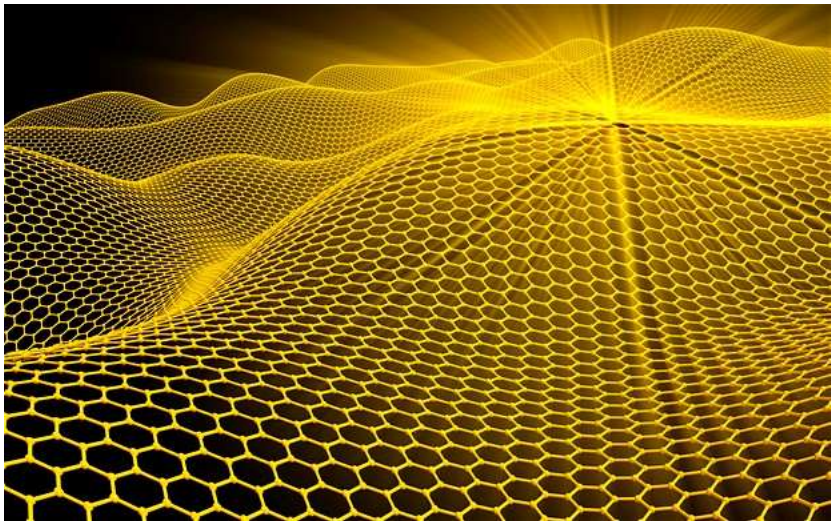
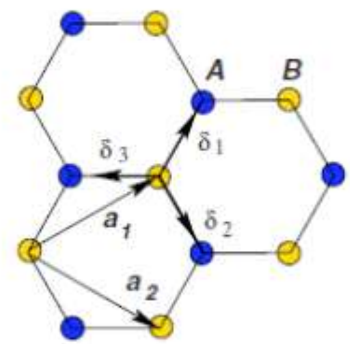
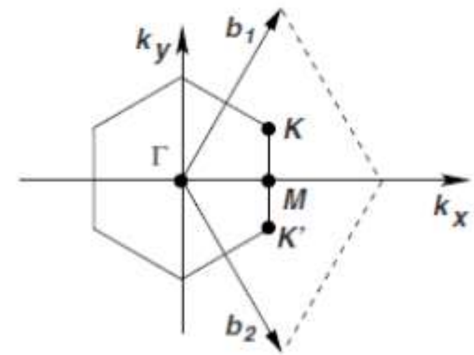
Quantum mechanics in real systems

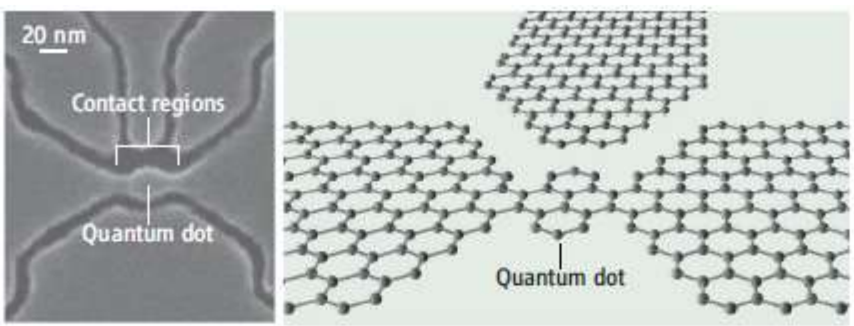
- Solution? Algorithms, but especially theory!!
- Hartree, Hartree-Fock, quantum chemistry
- Density-Functional Theory (DFT)
- 2014: researchers work hard to « better » solve quantum problems

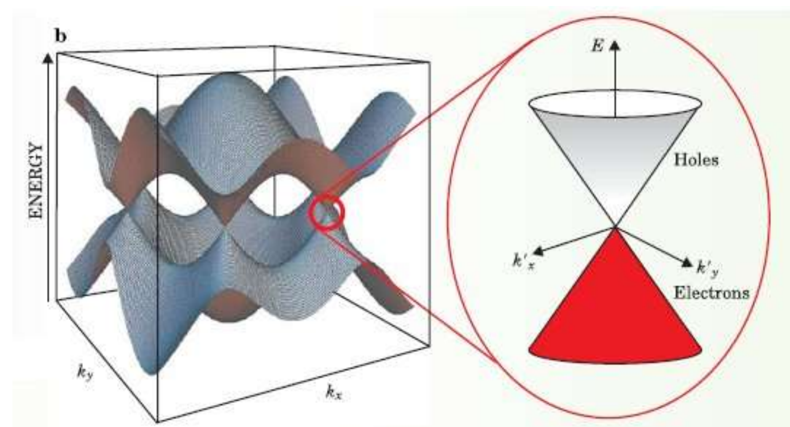
Quantum mechanics in real systems: graphene











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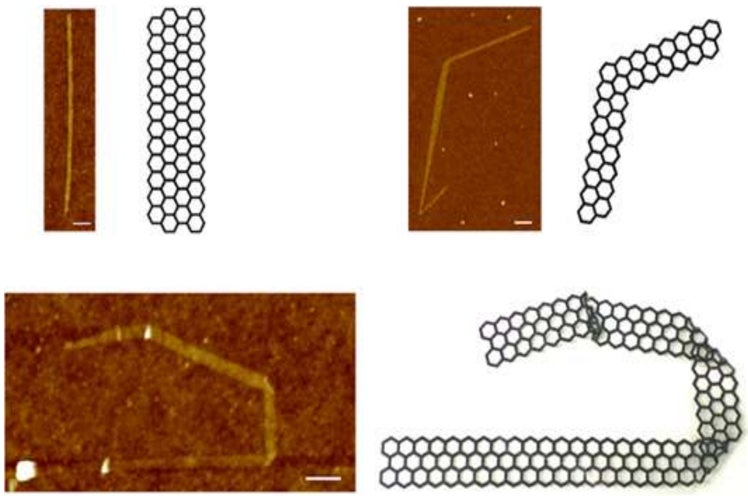
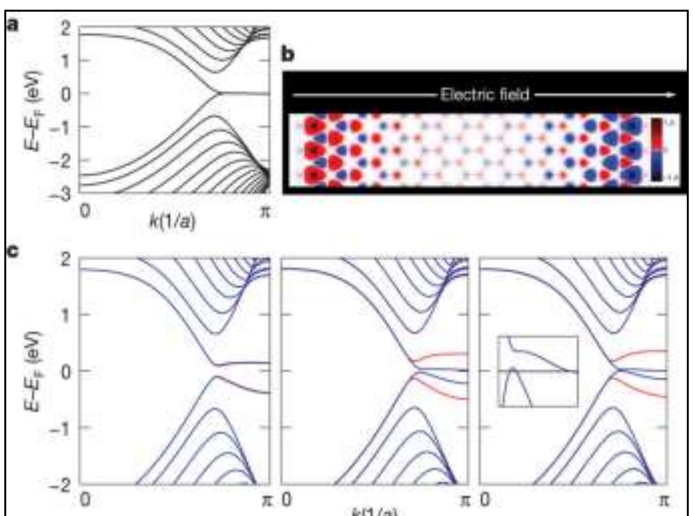
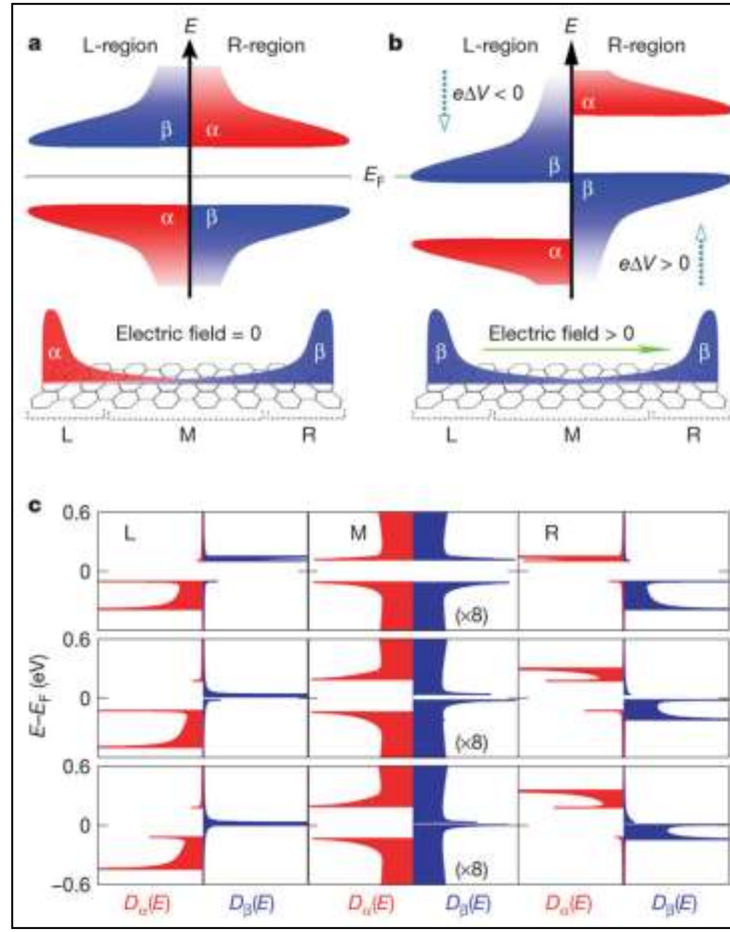
Quantum mechanics in real systems: graphene nanoribbons



Science 2008

Nature 2006





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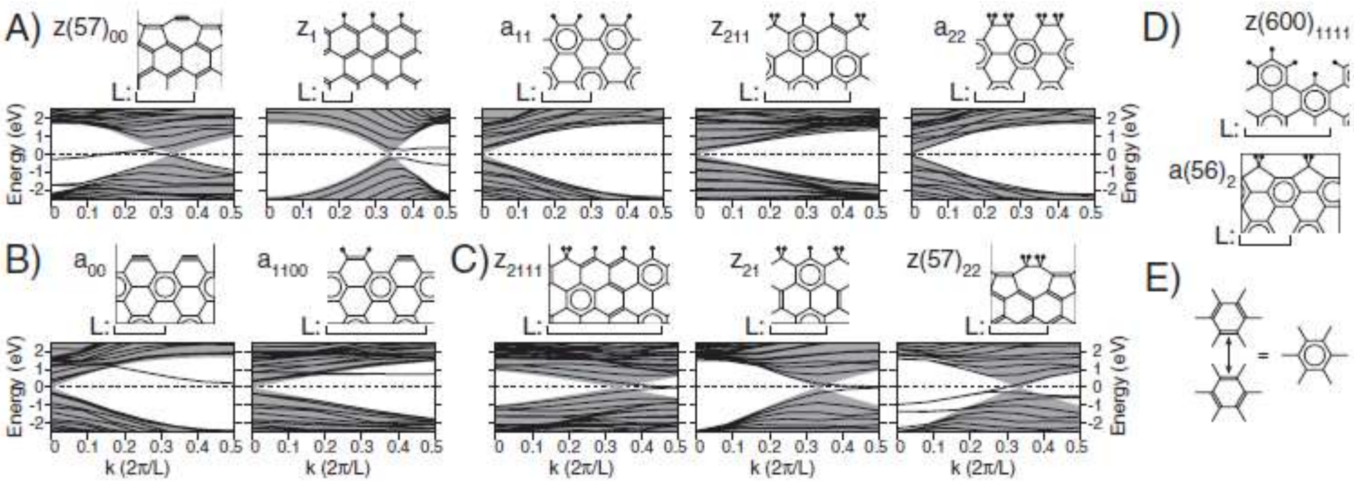
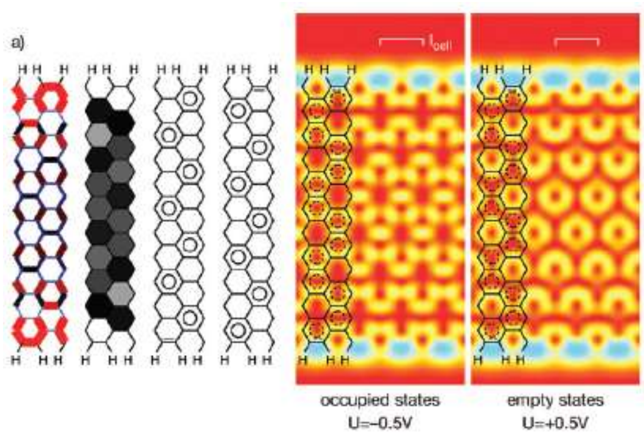
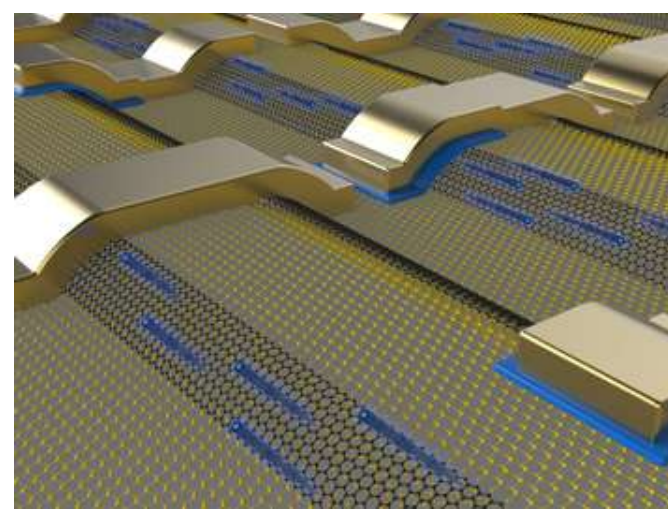


IMPMC, PRL 2008

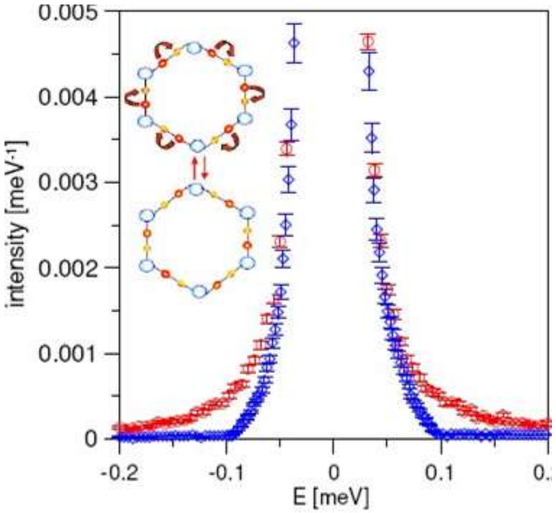
Nature 2014

IMPMC, JACS 2010

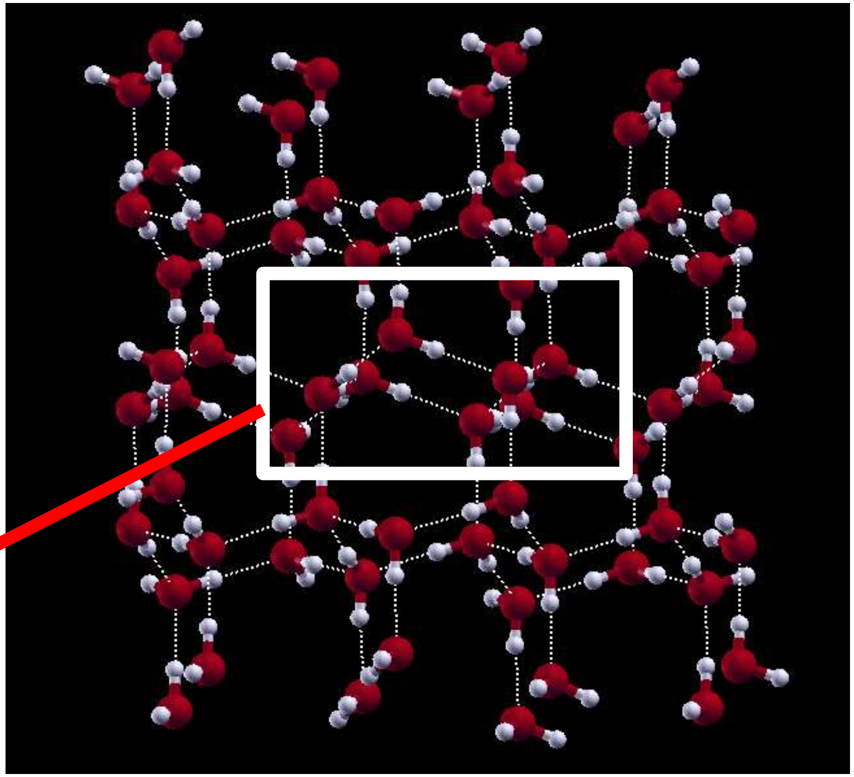


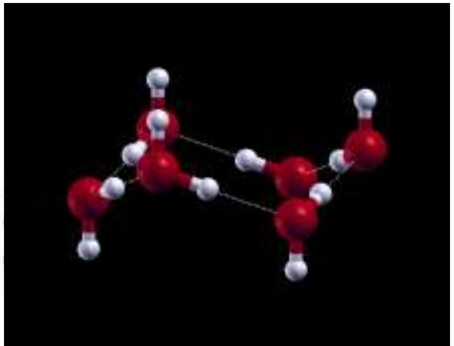


Quantum mechanics in real systems: quantum protons?

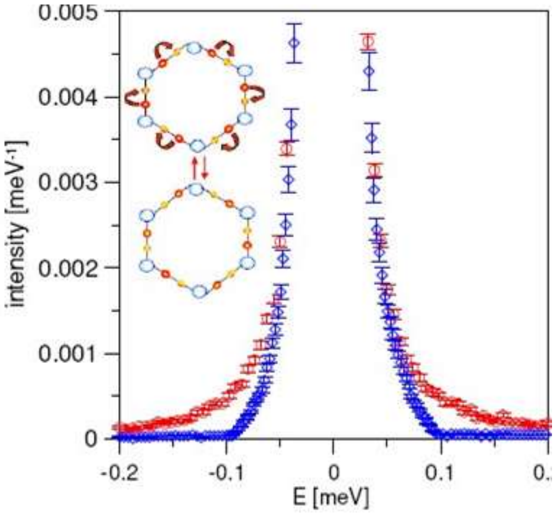


IMPMC, PRL 2009





Quantum mechanics in real systems: quantum protons?



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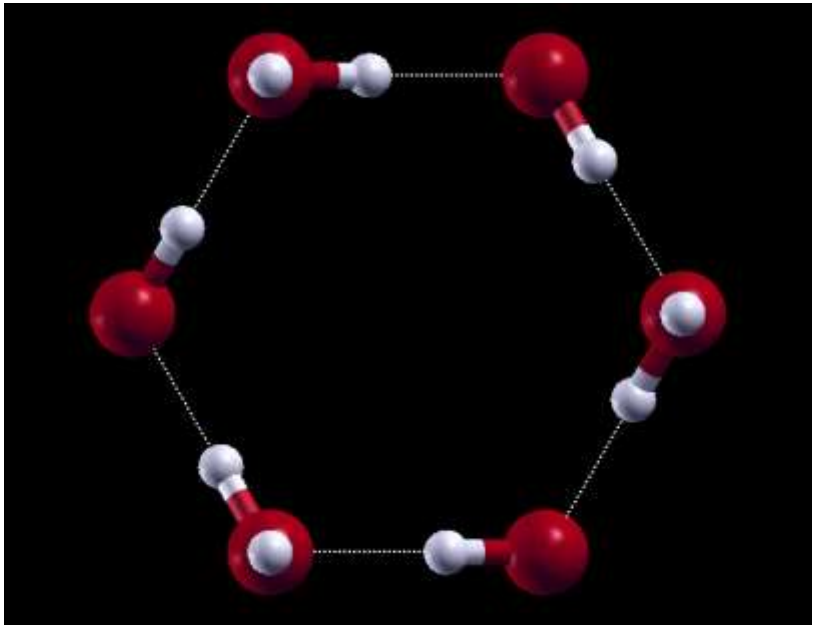
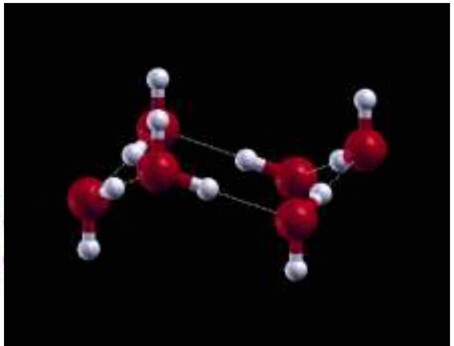
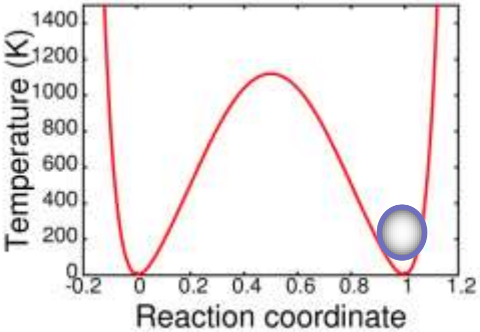
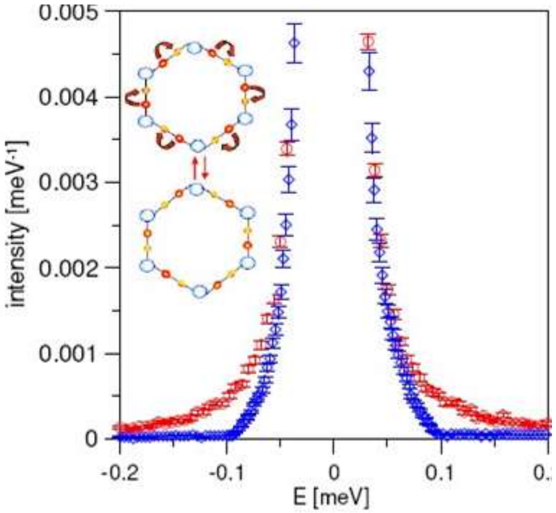


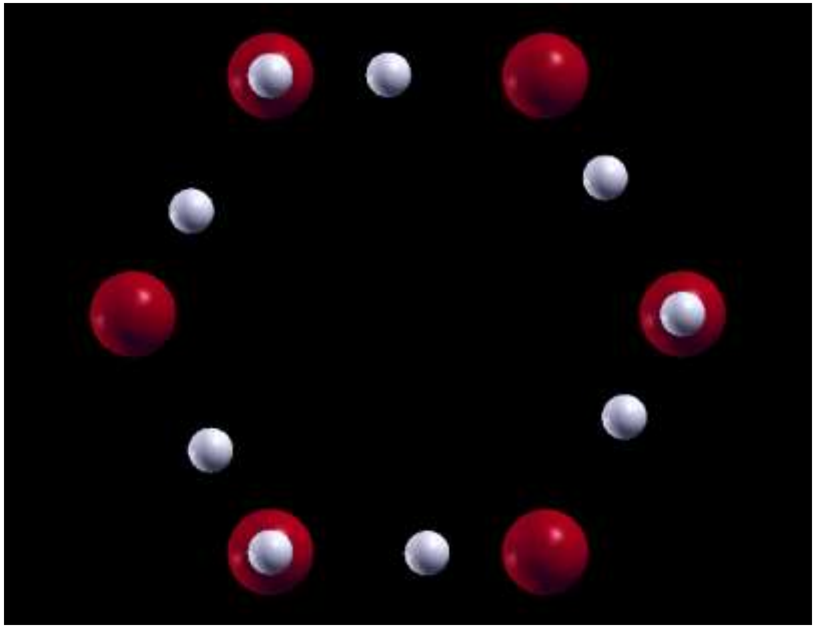


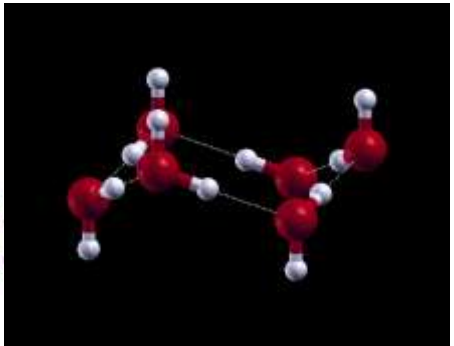


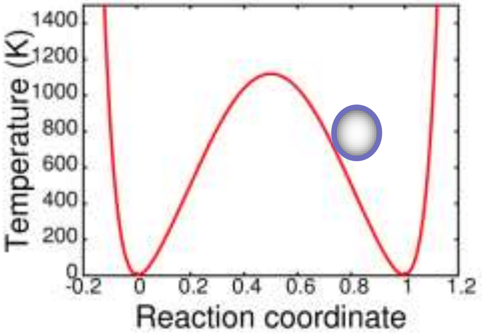
Quantum mechanics in real systems: quantum protons?



IMPMC, PRL 2009







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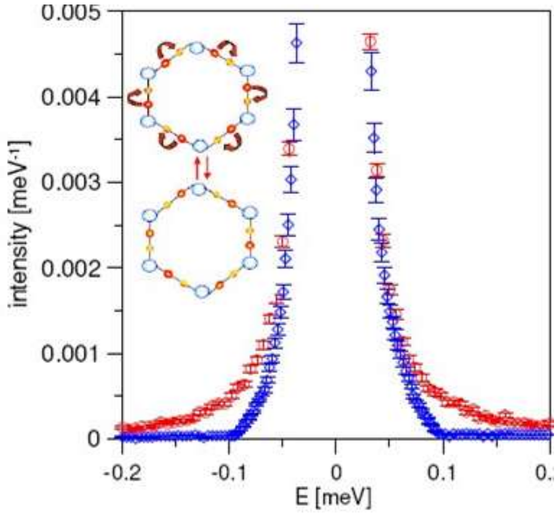
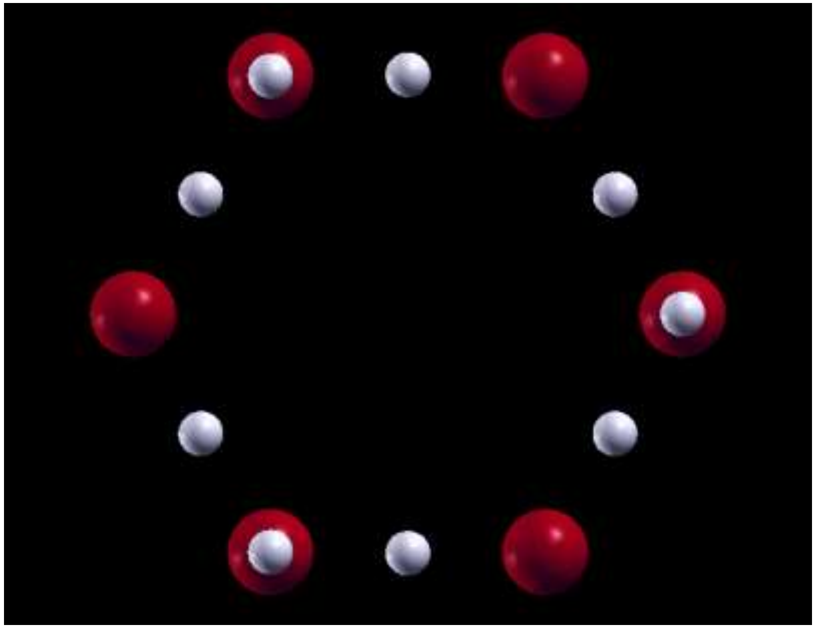
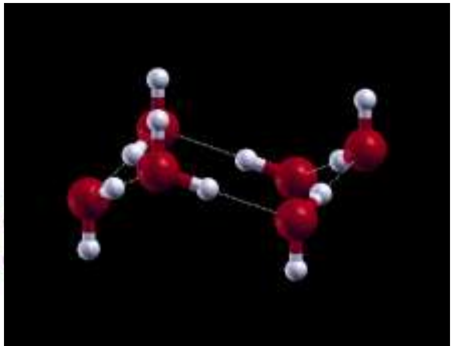
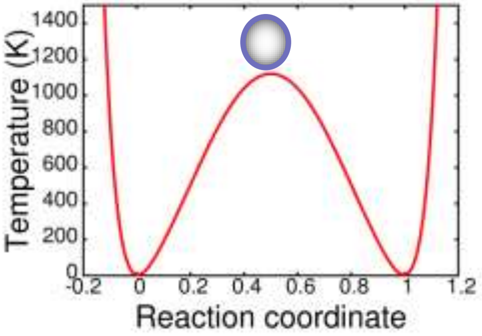
Quantum mechanics in real systems: quantum protons?



IMPMC, PRL 2009







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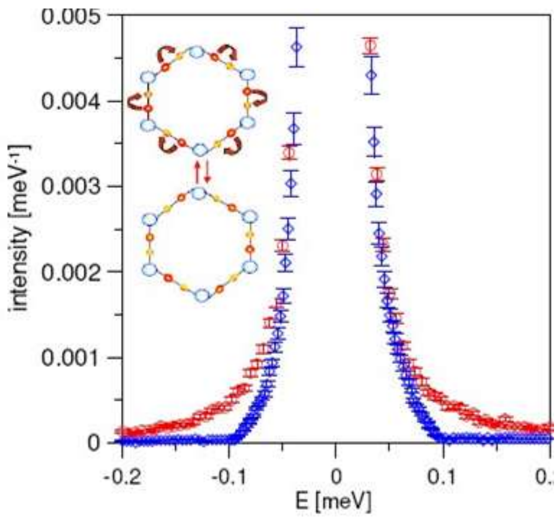
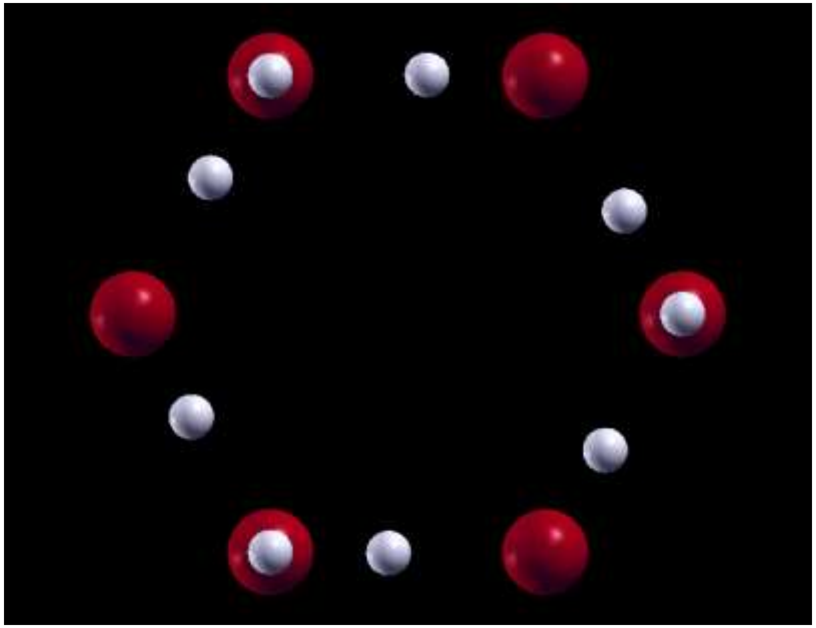
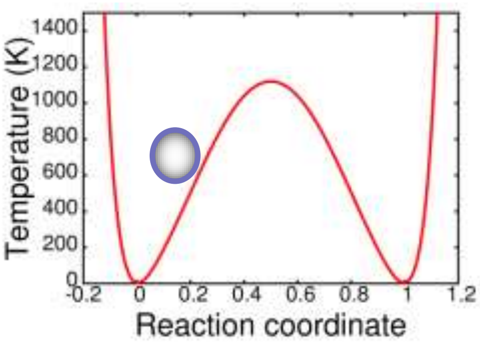
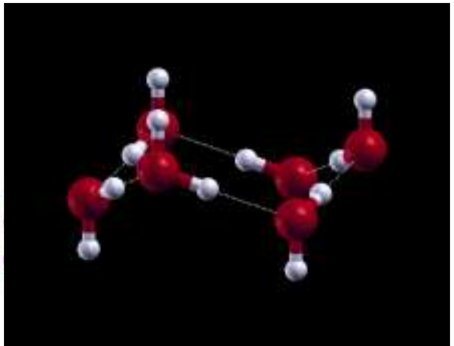
Quantum mechanics in real systems: quantum protons?



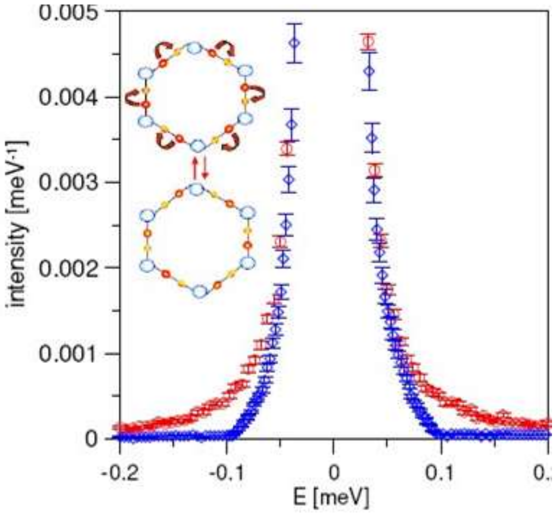
IMPMC, PRL 2009







Quantum mechanics in real systems: quantum protons?



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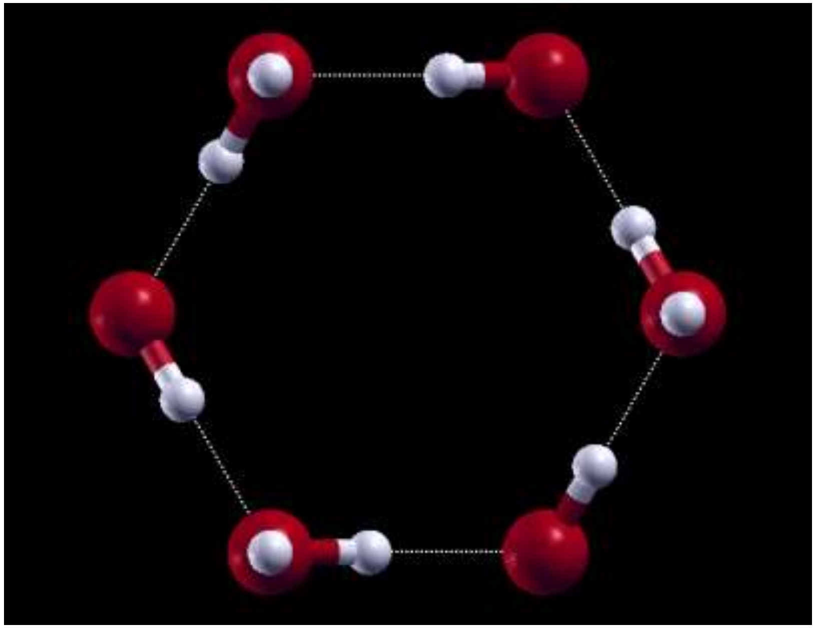

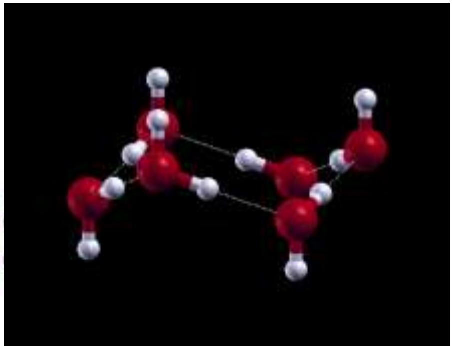

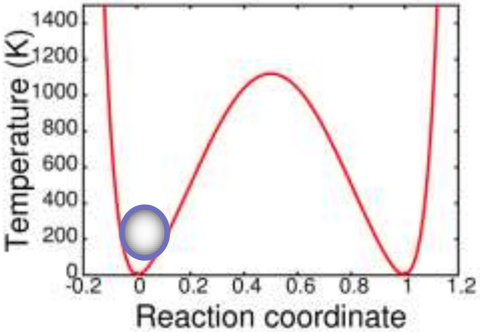

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Quantum mechanics in real systems

- Solution? Algorithms, but especially theory!!
- Hartree, Hartree-Fock, quantum chemistry
- Density-Functional Theory (DFT)
- 2014, researchers work hard to « better » solve quantum problems: Quantum Monte Carlo (IMPMC, JCTC2014), quantum proton (INSP/IMPMC, under review @PRL)

Thèse de F. Mouhat (ENS Chimie) – IMPMC/ENS

Thèse de M. Dagrada (M2 PCS) – IMPMC

Thèse de Y. Bronstein (M2 ICFP) – INSP/IMPMC

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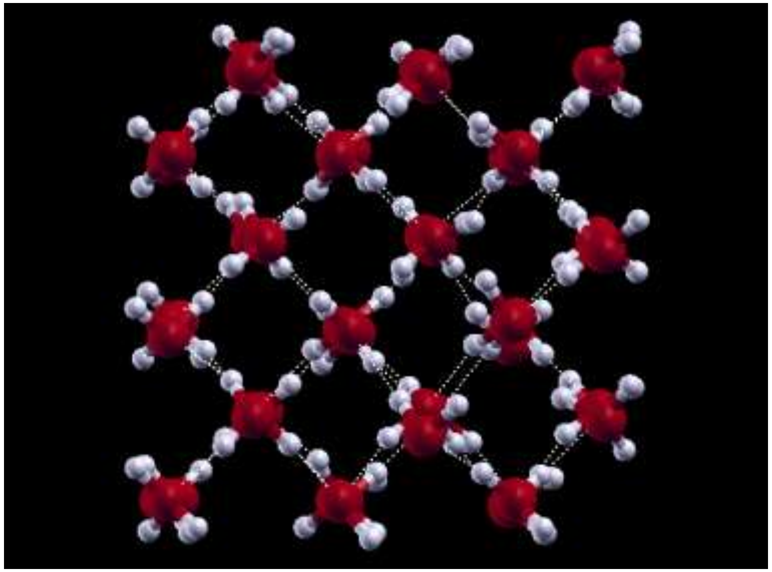
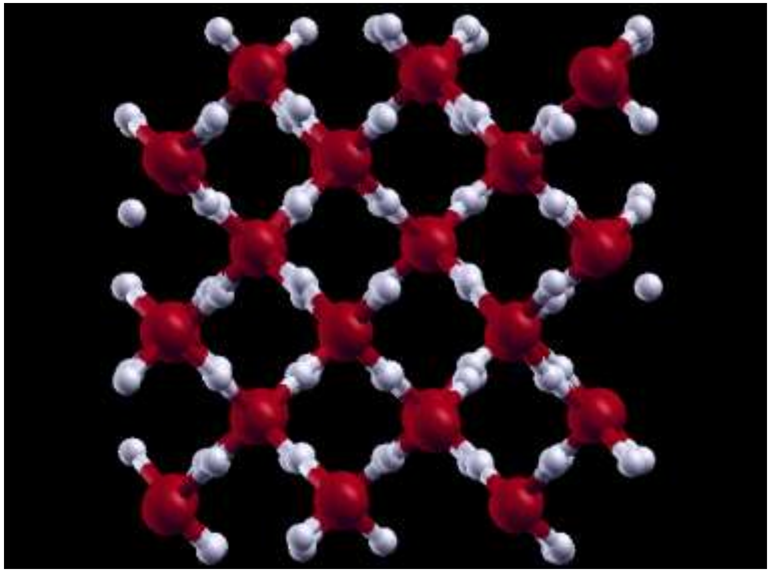
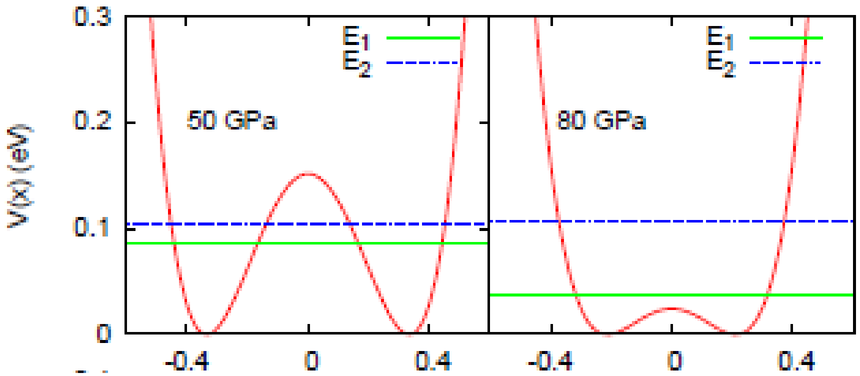
How to deal with quantum protons?



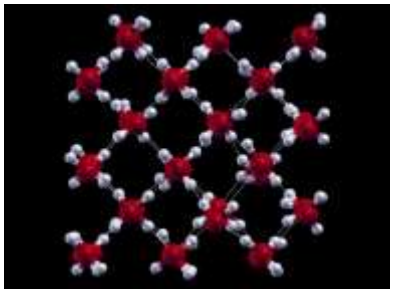
Ice VII, molecular



Ice X, symmetric



How to deal with quantum protons?



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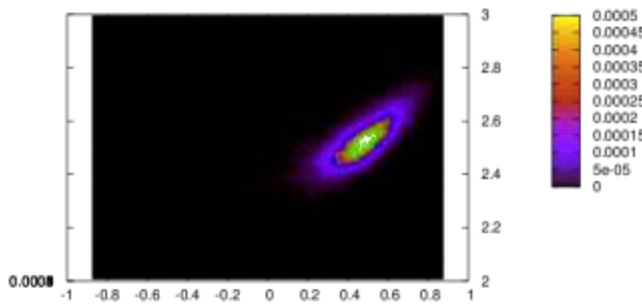

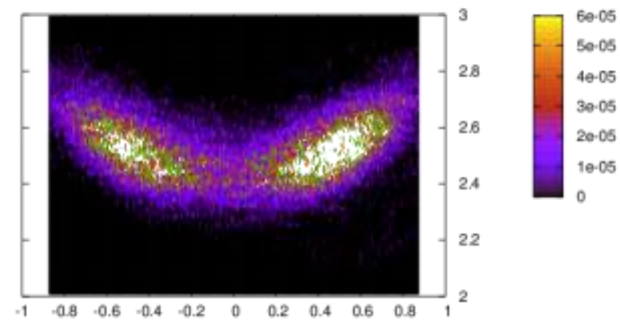

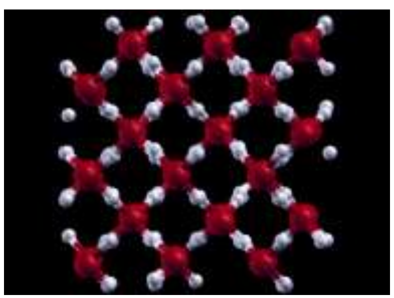

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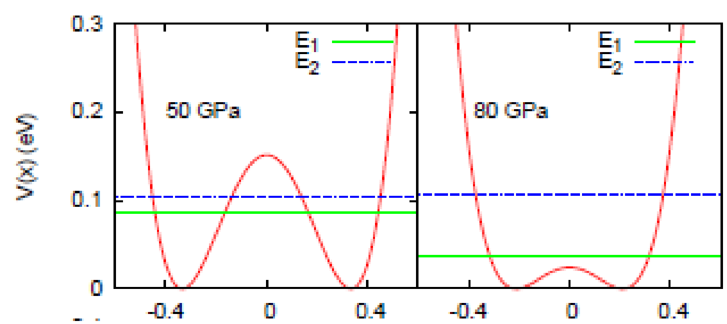

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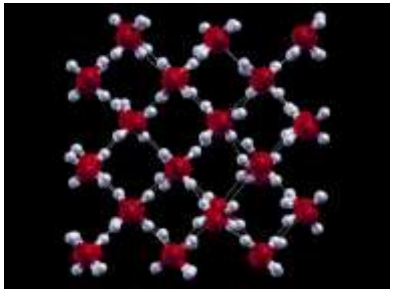

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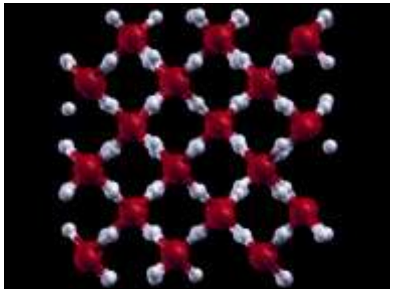

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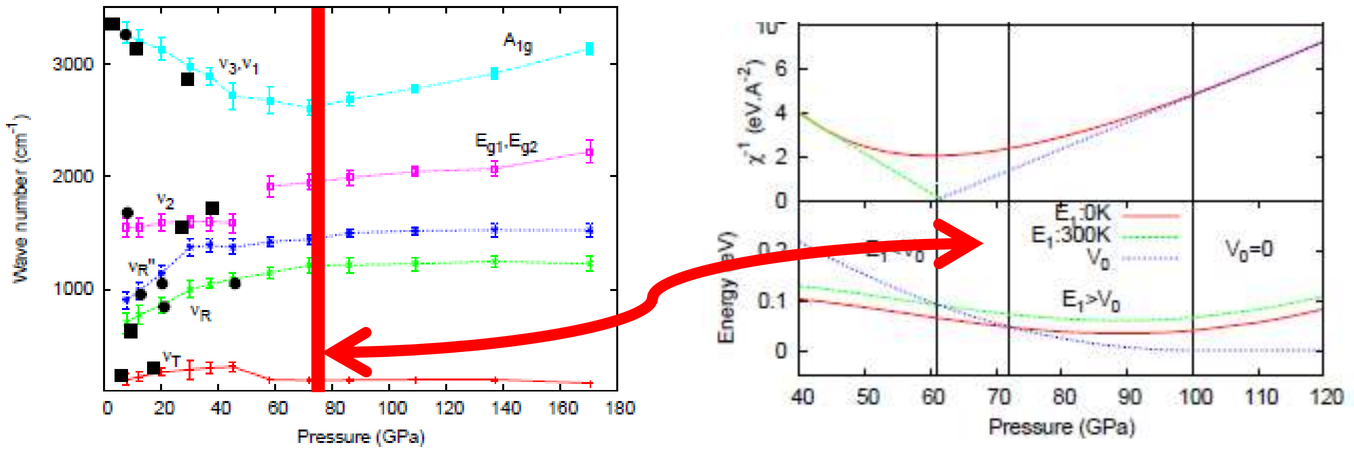
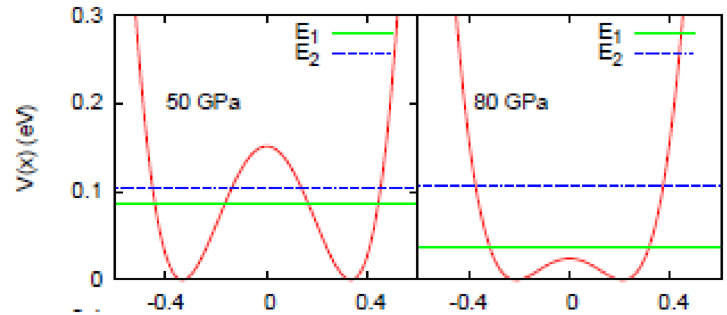
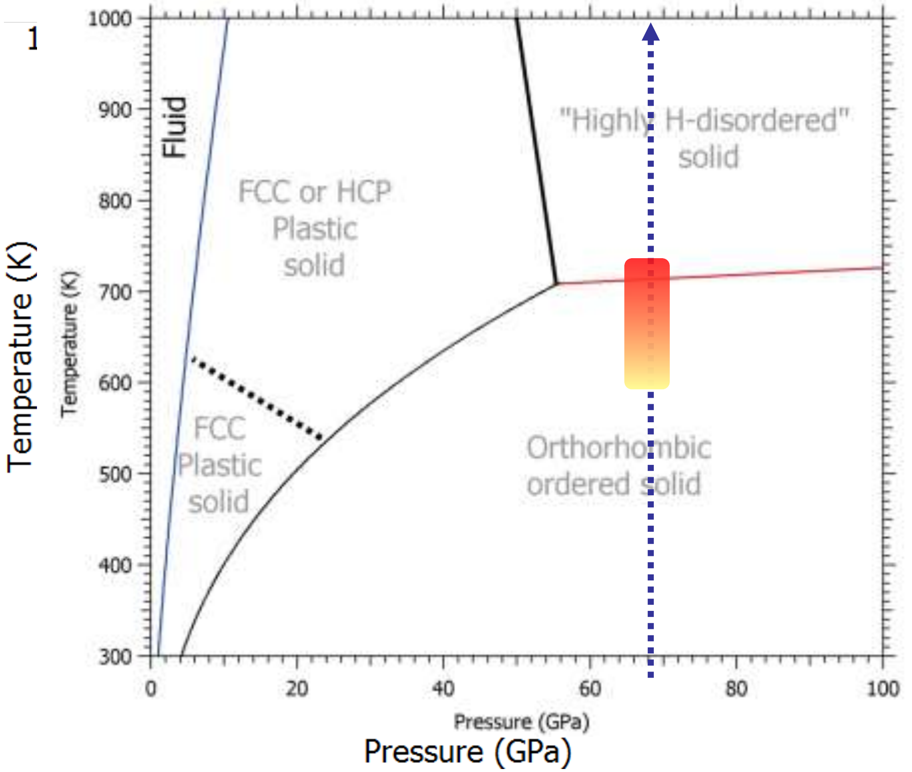


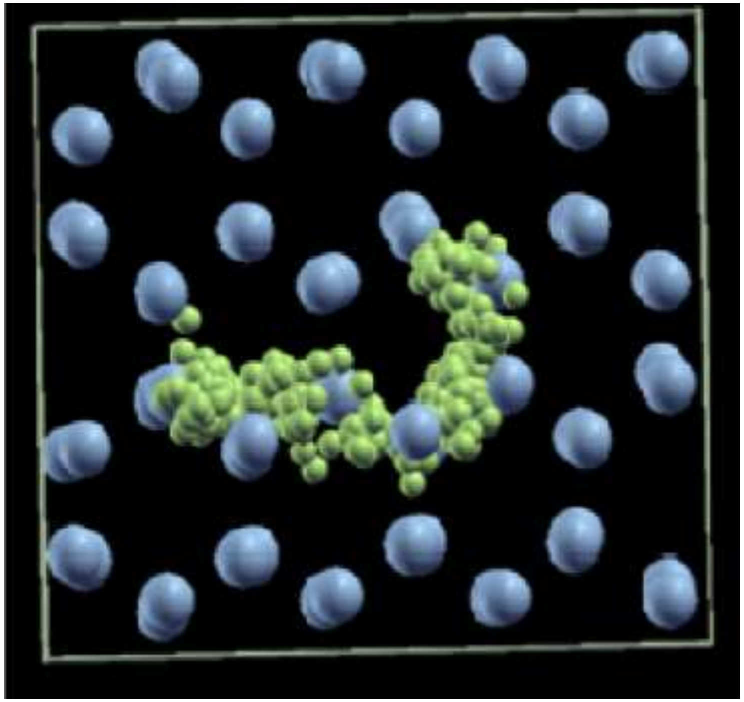
$$\chi = 2 \sum_{n \neq m} \frac{|\langle \Psi_n | x | \Psi_m \rangle|^2}{E_m - E_n}$$



H-bond ices at extreme conditions: ammonia

IMPMC Physics team (Ninet, Datchi, AMS)



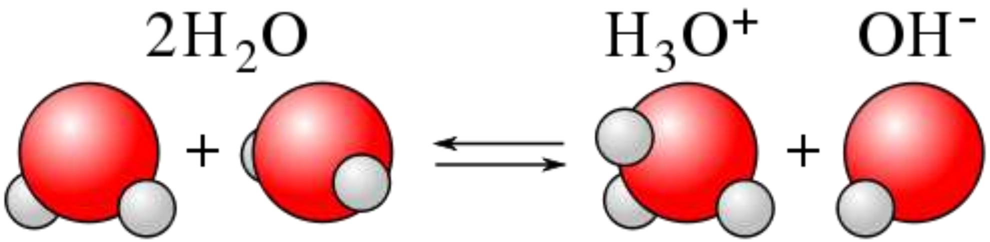


- Exp: discontinuity & disorder at high P/T
- Theory: superionicity at milder conditions
- New phase diagram & new challenges

Thèse de A. Mafety (M2 SMNO) - IMPMC

Ninet, Datchi, and AMS, Phys. Rev. Lett., (2012)

Autoprotolysis in water



- One of the most fundamental processes: pH

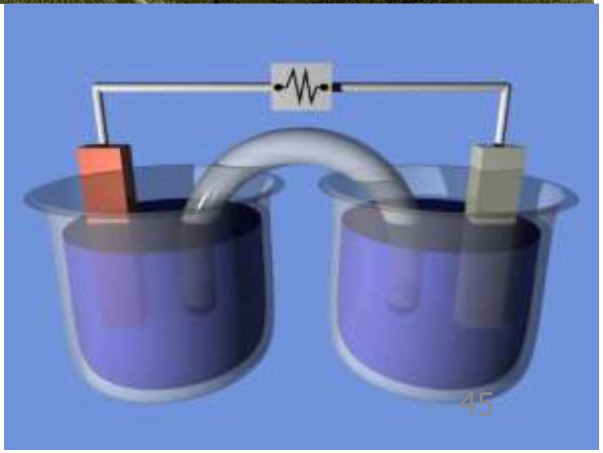
- Conductivity: 0.055 $\mu S \cdot cm^{-1}$

- K_w = 10^{-14} => 1 molecule dissociation over 10 hrs

Electrochemistry

- A milestone in the history of physics: Galvani, Nicholson, Volta, Faraday, Daniell, Arrhenius, Millikan, Brønsted…

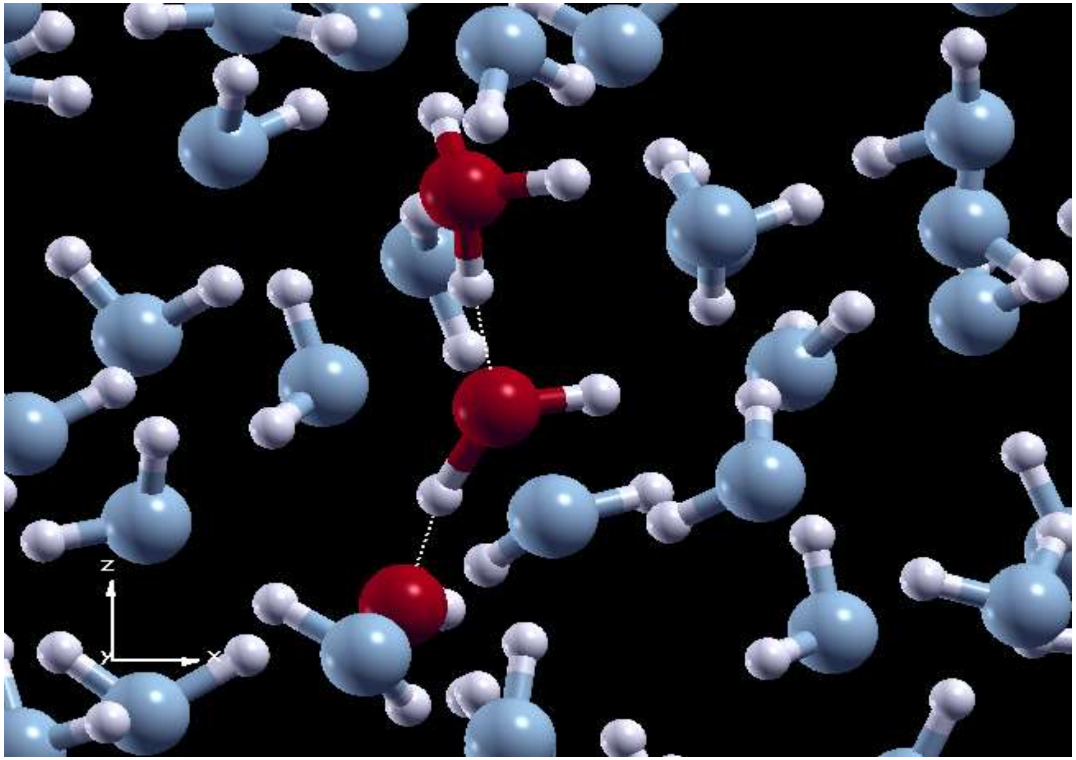
- Immense field of research: synthesis, materials processing, hydrogen/energy production, neurobiochemistry



- **No ab initio theoretical calculations!!**

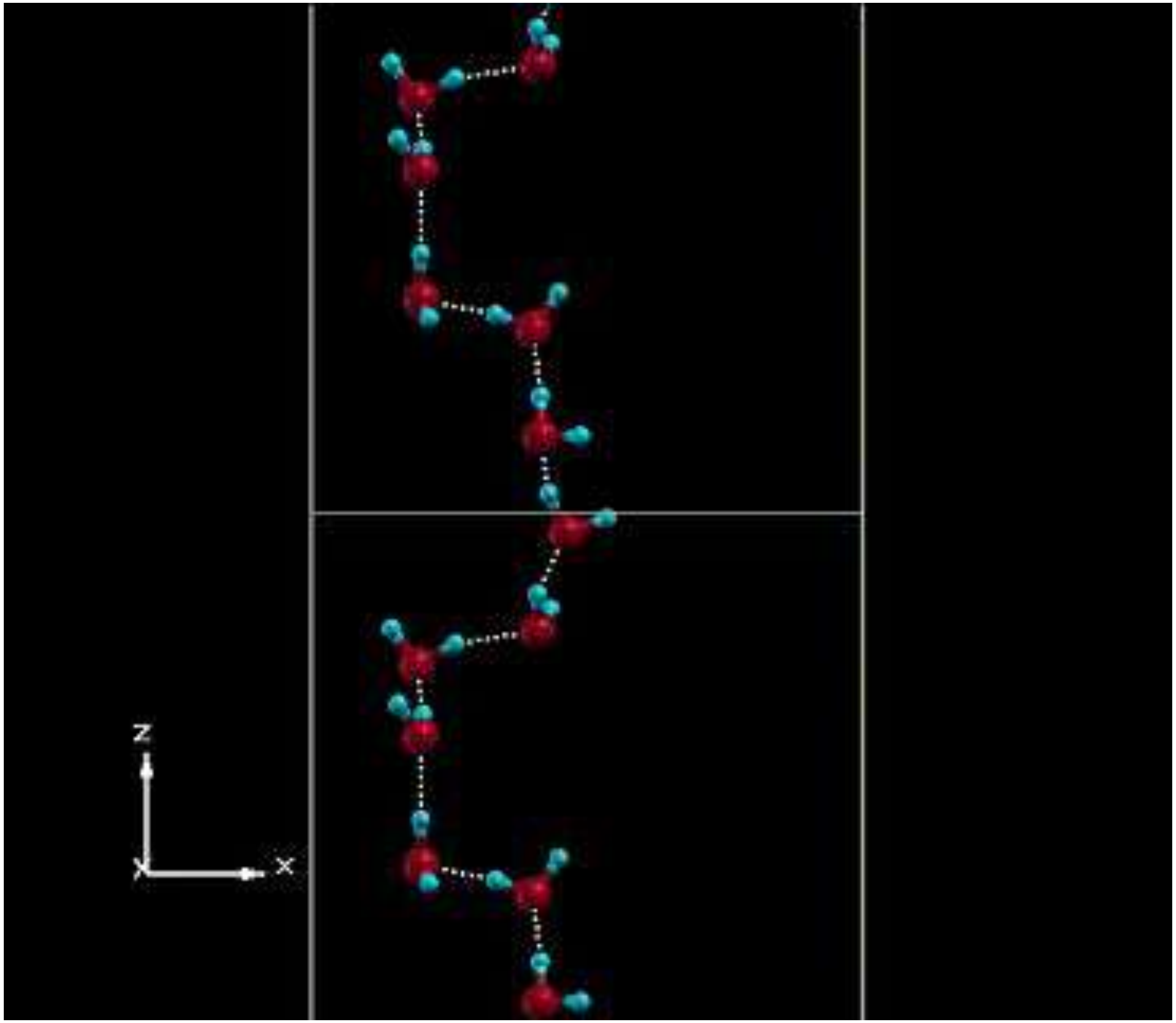
Field-induced dissociation

- Fields E ≥ 0.35 V/Å: protolysis; exp 0.3-0.6 V/Å (E.M. Stuve, CPL 2012, Cinam, APL 2013)



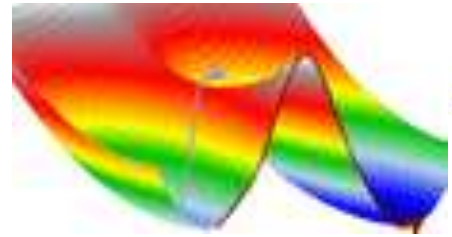
AMS, F. Saija, and P.V. Giaquinta, PRL 108, 207801 (2012)

Field-induced dissociation



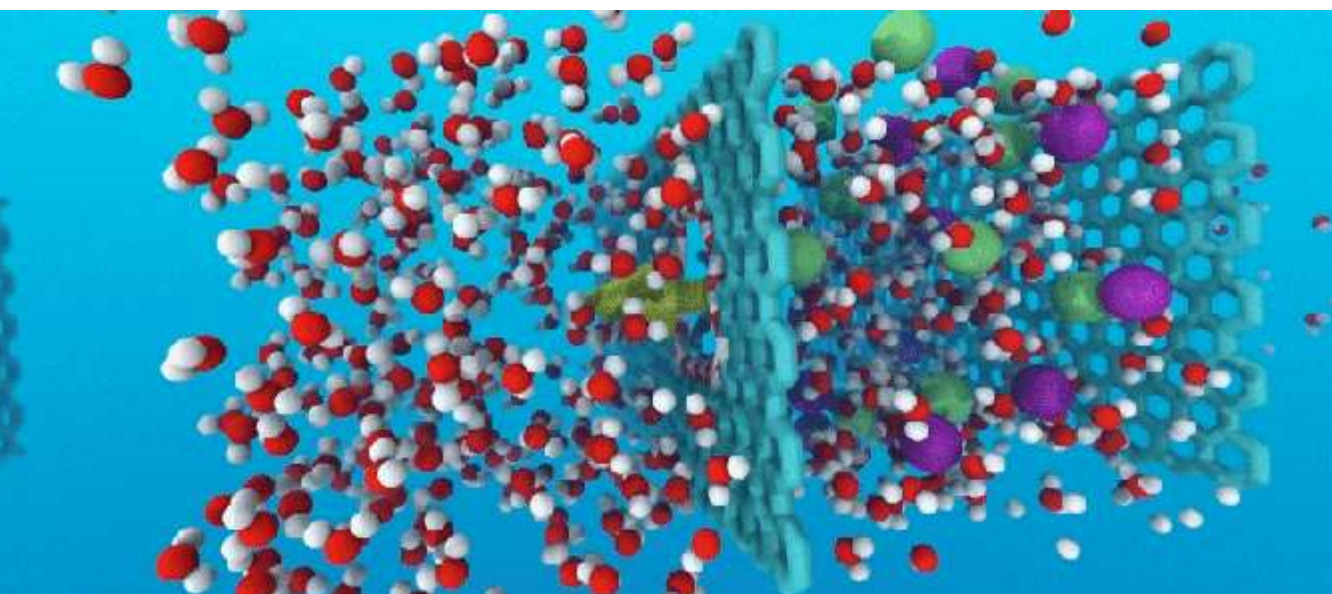
Thèses de S. Laporte (M2 NANOMAT) et de G. Cassone (M2 Italie)

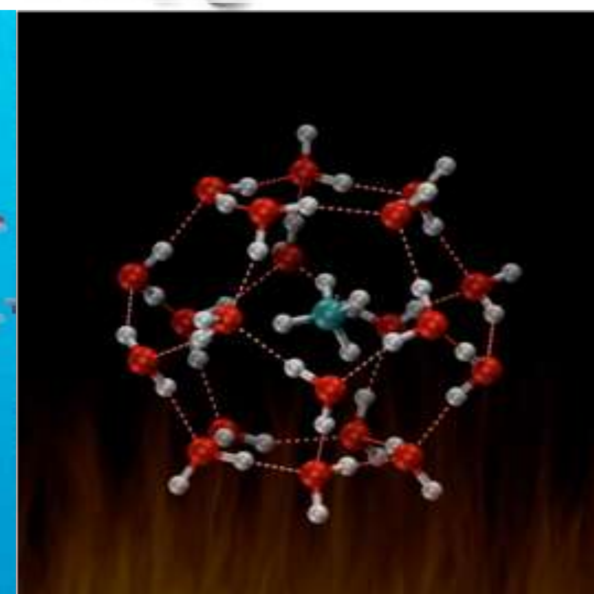
AMS, F. Saija, and P.V. Giaquinta, PRL 108, 207801 (2012)



Computational Materials Science, Physics and Chemistry

M2-Science des Matériaux et Nano-Objets/NANOMAT
M2-Chimie Théorique





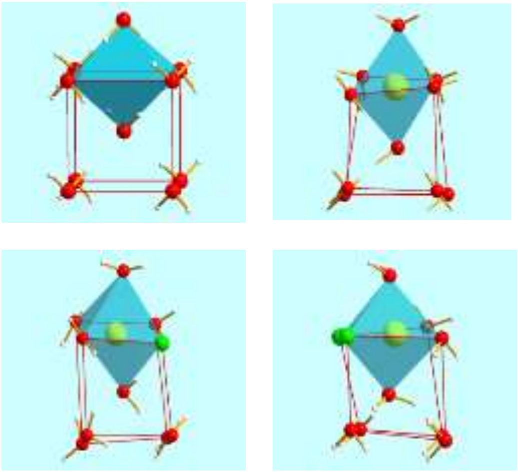
The teaching team

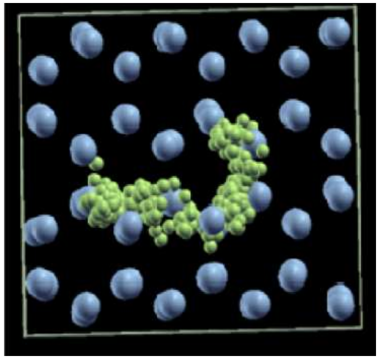
- A. Marco SAITTA – PR – CM/TD
- 43yr old
- PhD SISSA International School for Advanced Studies – Trieste, Italy
- Postdoc (3 yrs) University of Pennsylvania (Ivy League) – Philadelphia, USA
- MC at UPMC 2000-11
- PR at UPMC since 2011
- Deputy Dean of the Physics Faculty since Feb 2013

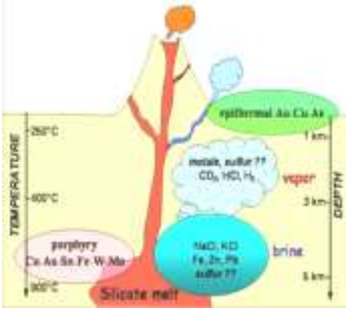
UPMC SORBONNE UNIVERSITÉS

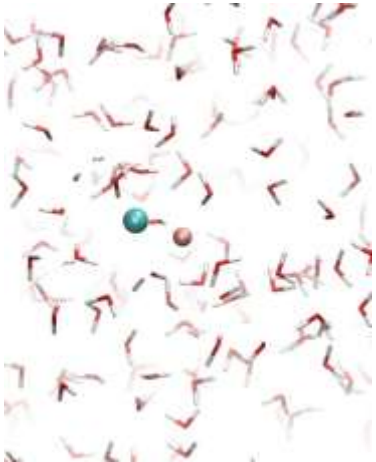
The teaching team

- **A. Marco SAITTA – Institut de Minéralogie et de Physique des Milieux Condensés**
- **Expertise : modelisation and computation in condensed matter physics, chemistry, materials science**
- **Main research areas:**
  - Water, ices, saline solutions
  - Other molecular systems: CO_2, NH_3
  - Precious metals in geological fluids
  - Graphene and nanotubes









The teaching team

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- Expertise : modelisation and computation in condensed matter physics, chemistry, materials science
- Main research areas:
  - Water, ices, saline solutions
  - Other molecular systems: CO_2, NH_3
  - Precious metals in geological fluids
  - Graphene and nanotubes
- Scientific production:
  - ~70 articles
  - 1 Nature, 2 Nature Materials, 1 PNAS (sept 2014), 18 Phys. Rev. Lett.
  - ~2300 citations, h-factor = 25

SORBONNE UNIVERSITÉS

The teaching team

- A. Marco SAITTA – PR

- Responsable UE LP329 – Physique Numérique (tronc commun L3 Licence de Physique)

- Responsable UE LP339 – Mécanique Quantique 3 – Cohésion de la Matière (option 2$^{\text{ème}}$ période, puis tronc commun L3 Licence de Physique)

- Since october 2013: Responsable UE NP446 – Computational Materials Science, M2 Science des Matériaux et des Nano-Objects (SMNO)/NANOMAT

Objectives of the course

- Introduce the conceptual framework and the main methods of computational investigation of atomistic condensed matter
  - Classical Molecular Dynamics
  - Ab initio Density Functional (+Perturbation) Theory
  - Quantum MC (Michele Casula)

- Propose a battery of computer lab « hands-on » projects

- Provide a flavor of theoretical (and experimental !) research @UPMC in condensed matter and chemical physics

Organisation of the course

- 8 Cours Magistraux, 3h each (MD, DFT, QMC)
- 2 TD + 2 TP (phonons in linear chain, electrons in periodic potential)
- 6 sessions for computational project, 3h each

Preliminary plan 2014-15

Semaine	Date				
3	18/09/14	Jeudi	8h30-10h	**CM1**	Introduction
			10h30-12h30	**TD1**	Linear chain oscillations
4	25/09/14	Jeudi	8h30-12h30	**TP1**	Linear chain oscillations
5	02/10/14	Jeudi	9h-12h	**CM2**	Statistical Mechanics/Classical MonteCarlo
	03/10/14	Vendredi	8h30-10h30	**TD2**	Electron(s) in a periodic potential
	03/10/14	Vendredi	11h-12h30	**CM3**	Molecular Dynamics
6	09/10/14	Jeudi	8h30-12h30	**TP2**	Electron(s) in a periodic potential
	10/10/14	Vendredi	8h30-10h30	**CM4**	Molecular Dynamics
	10/10/14	Vendredi	11h-12h30	**CM4**	Density Functional Theory
7	16/10/14	Jeudi	9h-12h	**CM5**	Density Functional Theory
	17/10/14	Vendredi	9h-12h	**CM6**	Density Functional Theory
8	23/10/14	Jeudi	9h-10h30	**CM7**	Density Functional Theory
	23/10/14	Jeudi	11h-12h30	**CM7**	Ab initio Molecular Dynamics
	24/10/14	Vendredi	9h-12h	**CM8**	Quantum Monte Carlo
9	30/10/14	Jeudi	9h-12h30	**Projet 1**	
10	06/11/14	Jeudi	9h-12h30	**Projet 2**	
11	13/11/14	Jeudi	9h-11h	**Examen**	
12	20/11/14	Jeudi	9h-12h30	**Projet 3**	
13	27/11/14	Jeudi	9h-12h30	**Projet 4**	
14	04/12/14	Jeudi	9h-12h30	**Projet 5**	
15	11/12/14	Jeudi	9h-12h30	**Projet 6**	
	22/01/15	Jeudi	9h-17h	**Soutenances**	
	23/01/15	Vendredi	9h-17h	**Soutenances**	

The projects

- 2-3 students on each project
- From semi-analytical work to massively parallel calculations with provided MD/DFT/QMC codes
- Written article-like report
- Oral conference-like presentation

Population 2013-14 (1ère année)

- 12 SMNO (y compris ESPCI/ENSCP)
- 3 Nanomat (M2 International)
- 2 ENS-Chimie (M2 Chimie Théorique)

Population 2014-

- ~12 SMNO
- ?? Nanomat (M2 International)
- 3 ENS-Chimie (M2 Chimie Théorique)

Computational Materials Science, Physics and Chemistry
M2-SMNO 2013-14

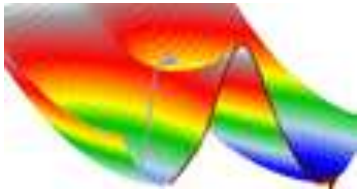
Félix Mouhat (M2 Chimie Théorique)
Normalien – Chimie ENS
felix.mouhat@clipper.ens.fr

« J'espère que nous serons amenés à rediscuter bientôt (de recherche ou de cours). En attendant, je vous signale que vos cours m'ont déjà servi à faire une remarque appréciée lors d'une conférence où une chercheuse présentait des calculs DFT couplés au modèle d'Ising. J'en suis donc ravi.

J'insiste également sur le fait qu'il ne faut jamais hésiter à me solliciter pour faire la publicité de votre cours, ou plus généralement du parcours TM du master SMNO. Vous pouvez citer mon adresse mail etc...
Je retourne à mes calculs de constantes élastiques en attendant votre réponse. »

Computational Materials Science, Physics and Chemistry

M2-SMNO/Nanomat
M2-Chimie Théorique



A. Marco Saitta

Professeur – IMPMC

marco.saitta@upmc.fr

LABoratoire d'EXcellence MATISSE