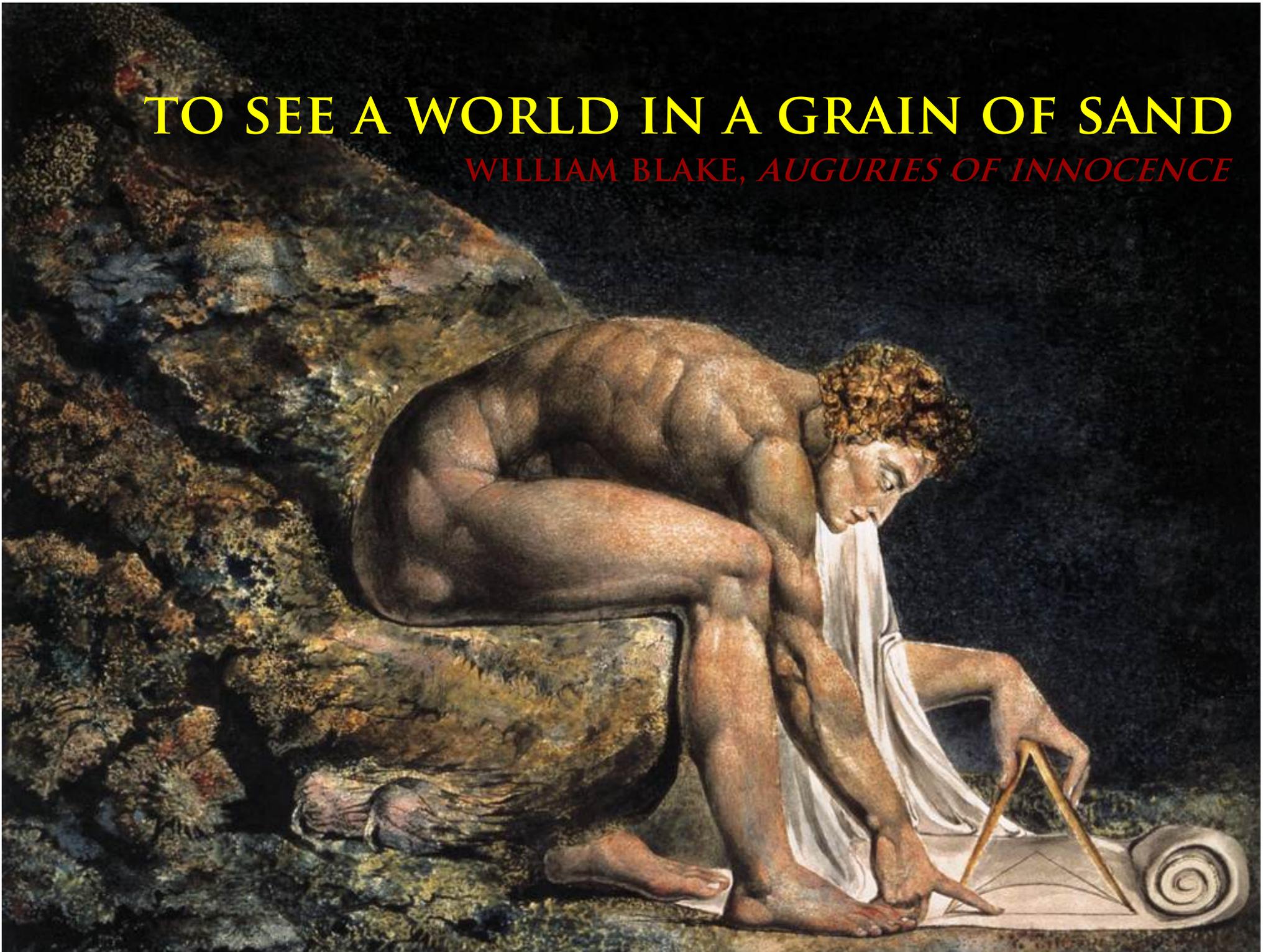


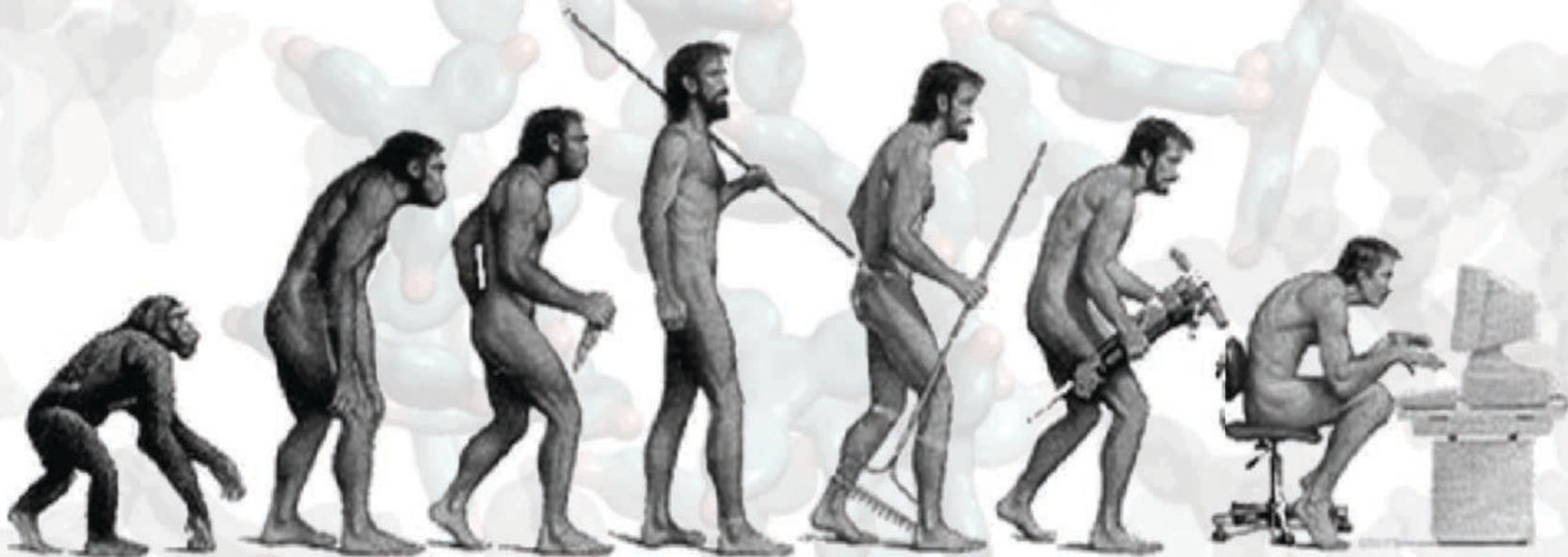
TO SEE A WORLD IN A GRAIN OF SAND

WILLIAM BLAKE, AUGURIES OF INNOCENCE



MATERIALS ARE KEY TO SOCIETAL WELL BEING

Human ages are named after materials:
stone, bronze, iron, nuclear, silicon...



MATERIALS ARE KEY TO SOCIETAL WELL BEING

We need novel materials for:

- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **High-tech and high-value industries**
- **Health care and biomedical engineering**
- **Pharmaceuticals** (crystallization, stability, polytypes)
- **Monitoring, provenance, and safety of foods**
- **Information and communication technologies**
- **Fundamental science** (graphene and 2D materials, topological insulators, entangled spins for quantum computing, high- T_c)
- **Experimental science** (detectors, sensors, magnets)

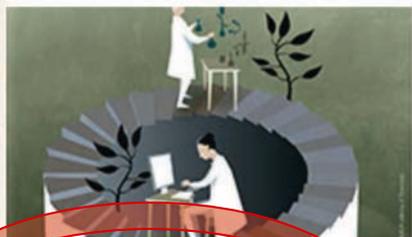


THE RISE OF MATERIALS SCIENCE



THE RISE OF SIMULATION SCIENCE

2013 Chemistry Prize



Taking the
Experiment to
Cyberspace

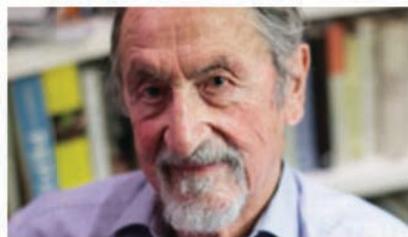


Photo © Harvard University

Martin Karplus

Martin Karplus, U.S. and Austrian citizen. Born 1930 in Vienna, Austria.



Photo: S. Fisch

Michael Levitt

Michael Levitt, U.S., British and Israeli citizen. Born 1947 in Pretoria,



Photo: Wikimedia Commons

Arieh Warshel

Arieh Warshel, U.S. and Israeli citizen. Born 1940 in Kibbutz Sde-

“The prize focuses on how to evaluate the variation in the energy of the real system in a accurate and efficient way [...]. **The Car–Parrinello approach is the leading strategy along this line.**”

“**Simulations are so realistic that they predict the outcome of traditional experiments.**”

From www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/



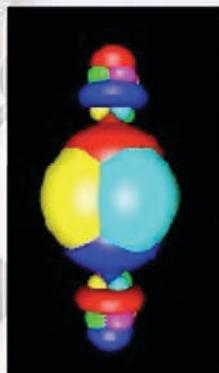
Inhomogeneous Electron Gas
P. Hohenberg and W. Kohn
Phys. Rev. **136**, B864 (9 November
1964)

Self-Consistent Equations Including
Exchange and Correlation Effects
W. Kohn and L. J. Sham
Phys. Rev. **140**, A1133 (15
November 1965)

Nobel Focus: Chemistry by Computer

21 October 1998

The 1998 Nobel Prize in chemistry recognizes two researchers whose work has allowed chemists to calculate the properties of molecules and solids on computers, without performing experiments in the lab. The basic principles of the calculation scheme were first described in *Physical Review* in the 1960s, and solid state physicists used them for decades before they became important in the chemistry world. The scheme drastically simplifies the solution of the quantum mechanical equations for a system of many electrons, and although approximate, the solutions are accurate enough that chemists can learn about large molecules without getting their hands wet.



Calculations made easy. Localized orbitals in the electronic structure of the BaTiO_3 crystal, calculated using density functional theory, which was invented by 1998 Nobel Laureate Walter Kohn.

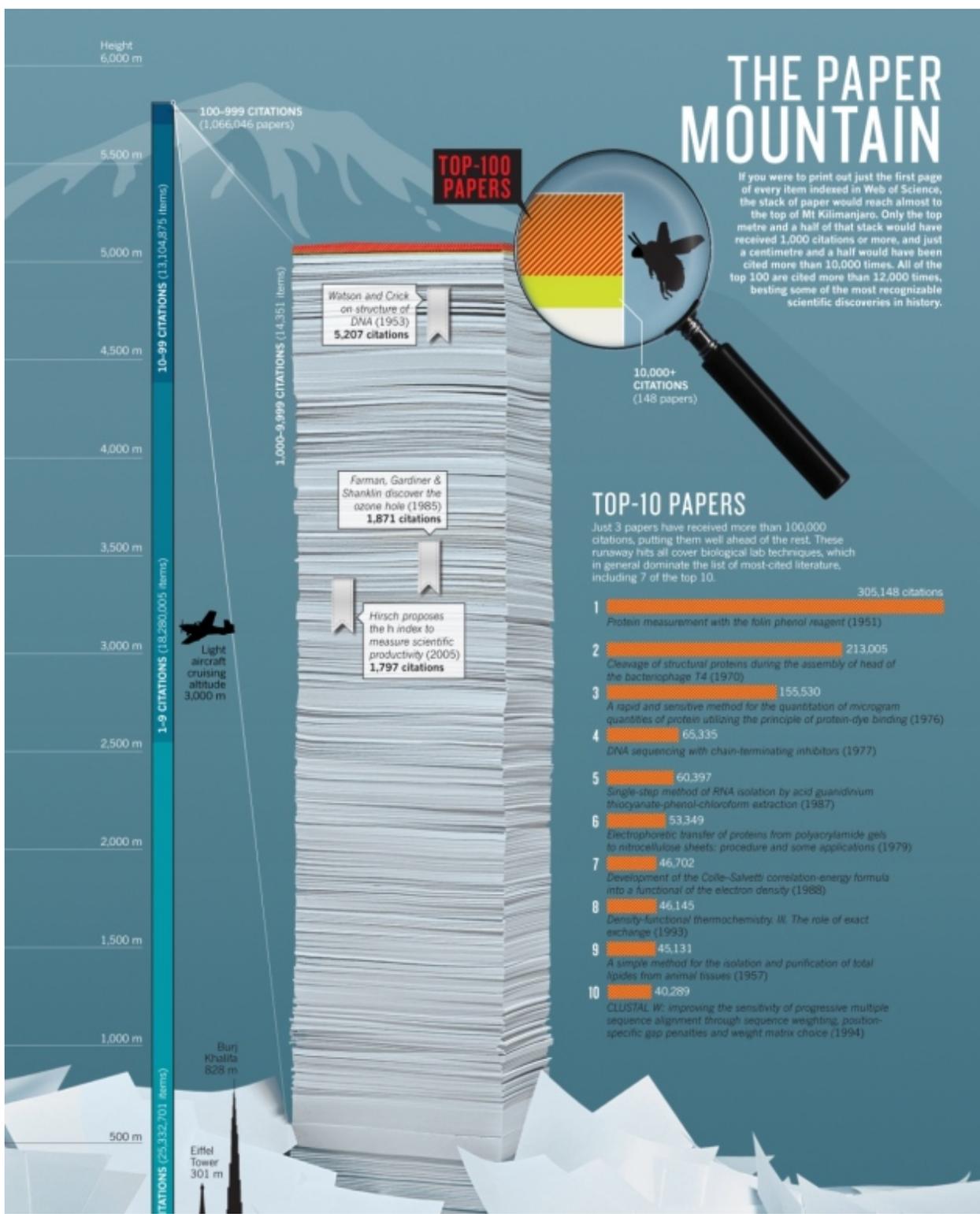
Nicola Marzari and David Vanderbilt/Rutgers University



MOST CITED PAPERS IN APS (FROM 1893)

	Journal	# cites	Title	Author(s)
1	PRB (1988)	39190	Development of the Colle-Salvetti Correlation-Energy ...	Lee, Yang, Parr
2	PRL (1996)	25452	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
3	PRA (1988)	22904	Density-Functional Exchange-Energy Approximation ...	Becke
4	PR (1965)	20142	Self-Consistent Equations Including Exchange and Correlation ...	Kohn and Sham
5	PRB (1996)	13731	Efficient Iterative Schemes for Ab Initio Total-Energy ...	Kresse and Furthmuller
6	PRB (1976)	13160	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1992)	10876	Accurate and Simple Analytic Representation of the Electron ...	Perdew and Wang
8	PRB (1999)	10007	From Ultrasoft Pseudopotentials to the Projector Augmented ...	Kresse and Joubert
9	PRB (1990)	9840	Soft Self-Consistent Pseudopotentials in a Generalized ...	Vanderbilt
10	PR (1964)	9789	Inhomogeneous Electron Gas	Hohenberg and Kohn
11	PRB (1981)	9787	Self-Interaction Correction to Density-Functional Approx. ...	Perdew and Zunger
12	PRB (1992)	9786	Atoms, Molecules, Solids, and Surfaces - Applications of the ...	Perdew, Chevary, ...
13	PRB (1986)	9313	Density-Functional Approx. for the Correlation-Energy ...	Perdew
14	PR (1934)	9271	Note on an Approximation Treatment for Many-Electron Systems	Moller and Plesset
15	PRB (1994)	9100	Projector Augmented-Wave Method	Bloch
16	PRL (1980)	7751	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder
17	PRL (1987)	7663	Inhibited Spontaneous Emission in Solid-State Physics ...	Yablonovitch
18	PRL (1986)	7589	Atomic Force Microscope	Binnig, Quate, Gerber
19	PRB (1991)	7425	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRB (1993)	6925	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
21	PR (1961)	6467	Effects of Configuration Interaction on Intensities and Phase Shifts	Fano
22	PR (1957)	6260	Theory of Superconductivity	Bardeen, Cooper, Schrieffer

THE PAPER MOUNTAIN



**NATURE,
October 2014**

**12 papers on DFT
in the top-100 most
cited papers in the
entire scientific
literature, ever.**

DFT reminder:

First Hohenberg-Kohn theorem

The density as the basic variable: the external potential V_{ext} determines uniquely the charge density, and **the charge density determines uniquely the external potential V_{ext} .**

1-to-1 mapping: $V_{\text{ext}} \iff \rho$

The universal functional $F[\rho]$

The ground state density determines the potential of the Schrödinger equation, and thus the wavefunction.

The universal functional F is well defined:

$$F[\rho(\vec{r})] = \left\langle \Psi \left| \hat{T} + \hat{V}_{e-e} \right| \Psi \right\rangle$$

Second Hohenberg-Kohn theorem

The variational principle – we have a *new Schrödinger's-like equation*, expressed in terms of the charge density only

$$E_v[\rho(\vec{r})] = F[\rho(\vec{r})] + \int v_{ext}(\vec{r})\rho(\vec{r})d\vec{r} \geq E_0$$

The Kohn-Sham mapping

F decomposed in non-interacting kinetic + Hartree + mystery

$$F[n(\mathbf{r})] = T_s[n(\mathbf{r})] + E_H[n(\mathbf{r})] + E_{xc}[n(\mathbf{r})],$$

Fermi's intuition: we construct E_{xc} using the **local density approximation** (at every point we use the XC energy density of the non-interacting homogenous electron gas at that density)

VOLUME 45, NUMBER 7

PHYSICAL REVIEW LETTERS

18 AUGUST 1980

Ground State of the Electron Gas by a Stochastic Method

D. M. Ceperley

National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, California 94720

and

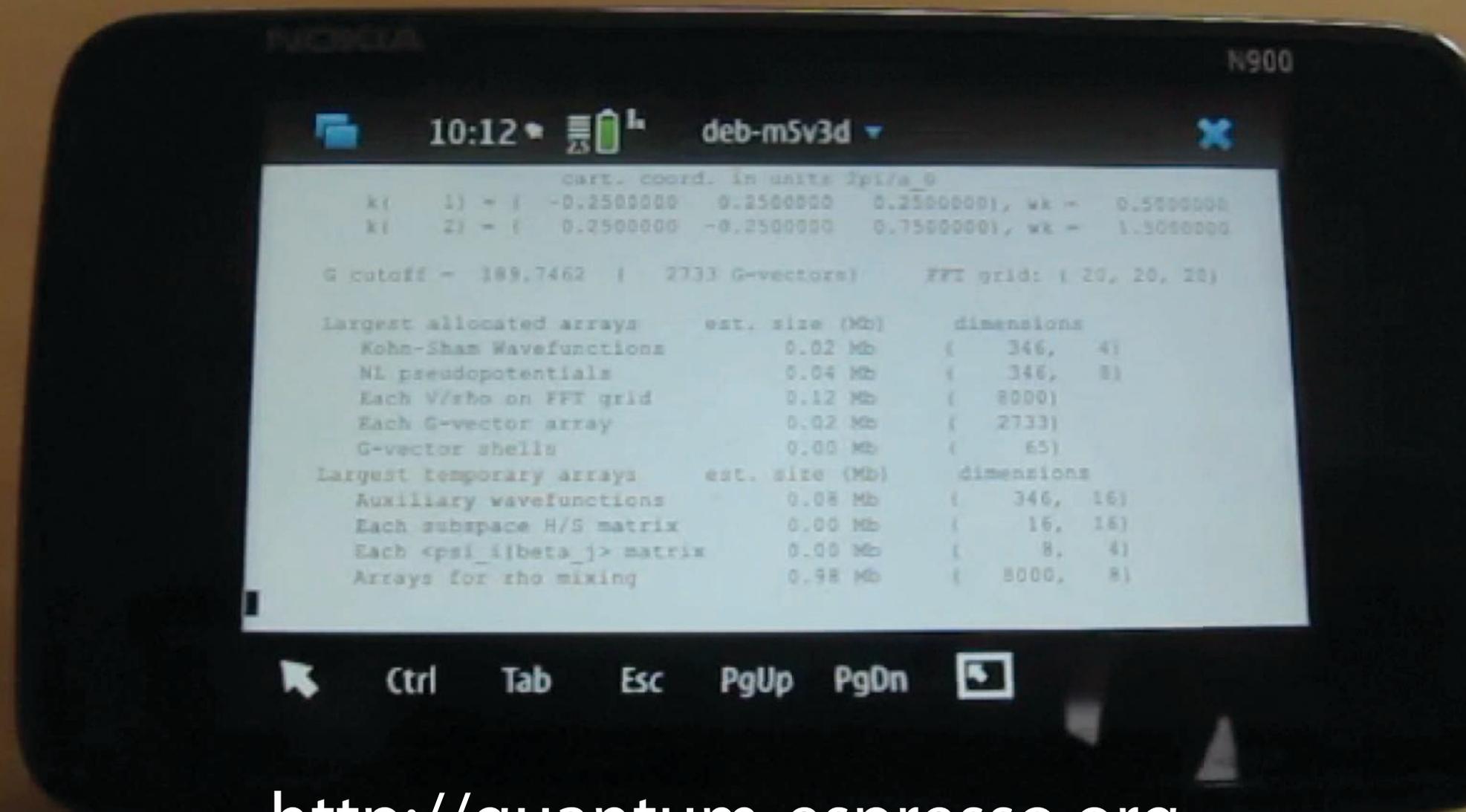
B. J. Alder

Lawrence Livermore Laboratory, University of California, Livermore, California 94550

(Received 16 April 1980)

An exact stochastic simulation of the Schroedinger equation for charged bosons and fermions has been used to calculate the correlation energies, to locate the transitions to their respective crystal phases at zero temperature within 10%, and to establish the stability at intermediate densities of a ferromagnetic fluid of electrons.

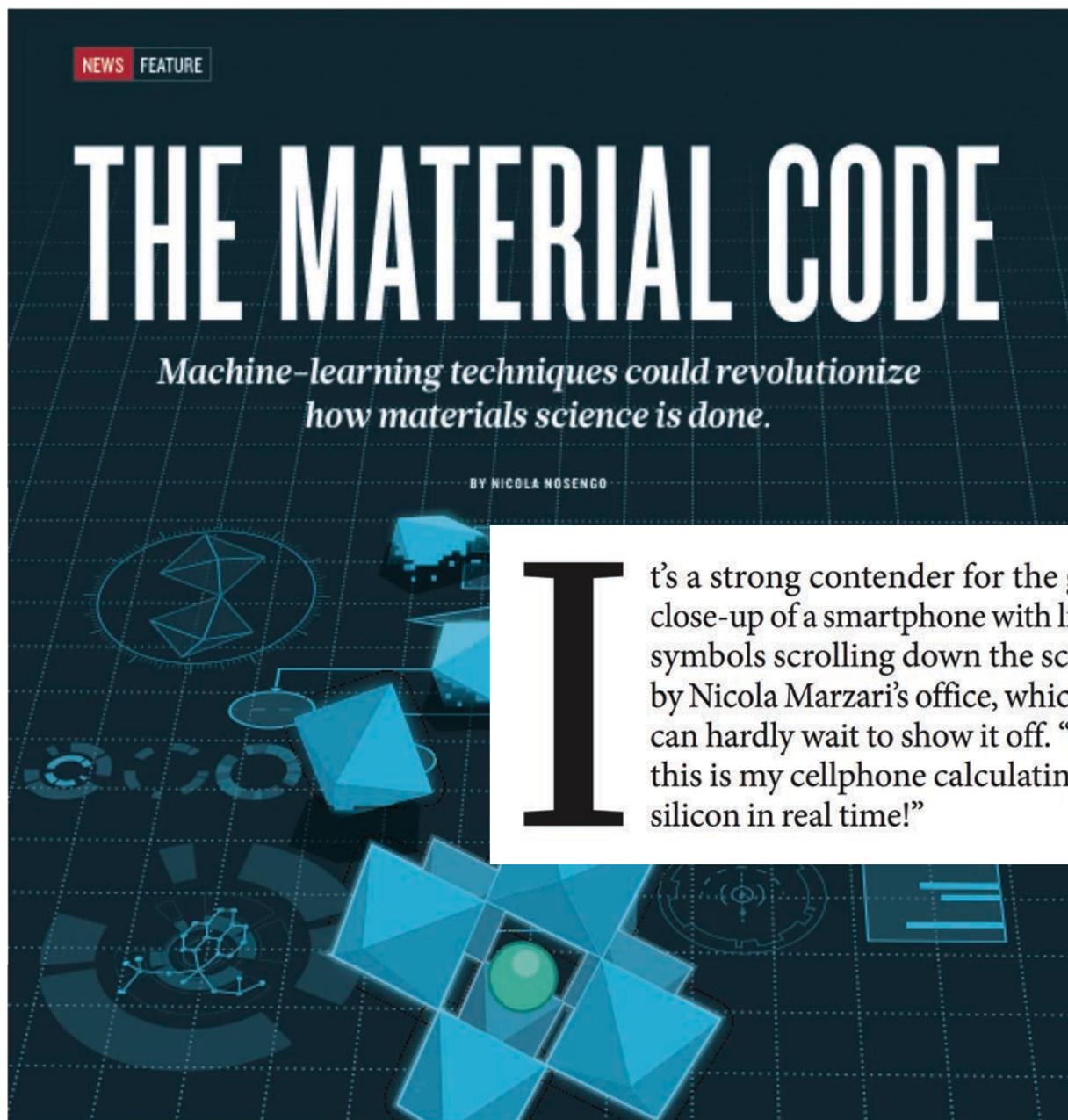
MY BEST CALCULATION: 2 NOV 2010



<http://quantum-espresso.org>



A SMALL STEP FOR A CELLPHONE, A GIANT LEAP FOR COMPUTERKIND



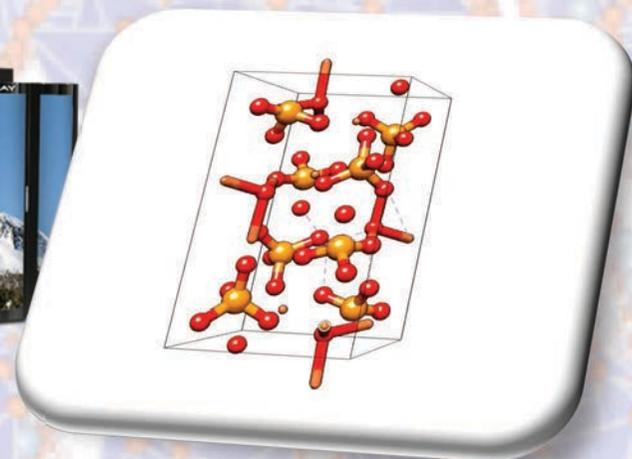
Nature, 5 May 2016



HIGH-THROUGHPUT SCREENING OF NOVEL MATERIALS

The number of inorganic materials known in full (i.e. with published structures) is **~200,000**

Currently, basic properties can be calculated on the entire Piz Daint CSCS supercomputer (3th in the world) at the tune of **1000 structures/minute**.



GREAT ENTHUSIASM FOR MATERIALS DISCOVERY

nature materials **REVIEW ARTICLE**
PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

nature chemistry **REVIEW ARTICLE**
PUBLISHED ONLINE: 19 MARCH 2009 | DOI: 10.1038/NCHEM.121

Towards the computational design of solid catalysts

LETTERS

Where are nature's missing structures?



Viewpoint: Materials Prediction Scores a Hit

Filip Ronning and John L. Sarrao, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Published October 7, 2013 | Physics 6, 109 (2013) | DOI: 10.1103/Physics.6.109

Calculations predicting a new high-pressure superconductor are borne out by experiment.

editorial

Fuelling discovery by sharing

GRC Gordon Research Conferences

7:40 pm - 9:30 pm

Structural Predictions at Extreme Conditions: Are Experiments Still Necessary?

Discussion Leader: John Tse (University of Saskatoon)



MAJOR EFFORTS WORLDWIDE

2011 – US: the Materials Genome Initiative

Materials Project (Berkeley), SUNCAT (Stanford), AFLOW (Duke), CHiMaD (NIST)

2014 – CH: **18 MCHF** MARVEL (Computational Design and Discovery of Novel Materials)

2015 – UK: **8.6 MGBP**, Materials Computational Discovery Centre, U. Liverpool

2015 – H2020: **14 M€**, Centres of Excellence on materials' simulations:

E-CAM – Simulation and Modelling; MaX – Materials Design at the Exascale;
NoMaD – Novel Materials Discovery

2015 - US DOE: **60 M\$**, 5 Centers on Comp. Materials Science, 4 years renewable:

U. Chicago, UC Berkeley, Rutgers, ORNL, USC

2016 – DK: **22 M\$**, Villum Centre for the Science of Sustainable Fuels and Chemicals (DTU Lyngby and Stanford)

2016 – US NSF: **35 M\$**, 2 Institutes on Scientific Software, 5 years: MolSSI (Stony Brook), Molecular Sciences Software Institute; SGCI (US San Diego) Science Gateways Community Institute

2017 - US Simons Foundation, **15 M\$/year**, Center on Computational Quantum Physics

2017 - US Toyota Research Institutes, **35 M\$**, Predictive Battery Performance



MARVEL MISSION STATEMENT

**Accelerated design and discovery of novel materials
via a materials' informatics platform of
high-throughput simulations, powered by**

- 1. advanced quantum simulations**, for accuracy
- 2. innovative sampling methods**, to explore materials space
- 3. materials informatics**, to leverage data, machine learning

**Materials for energy harvesting, storage, and conversion;
ICT; high value/high tech, and organic crystals/pharma.**



PHASE I 2014-18 (12 INST, 23 COMP, 3+15 EXP)

EPFL

ETHZ

PSI

IBM

UNIZH

UNIBAS

EMPA

UNIBE

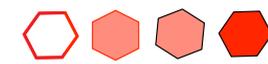
UNIFR

USI

CSCS

UNIGE

+ 15 experimental groups at
PSI, EMPA, UNIGE, EPFL



MATERIALS MODELLING

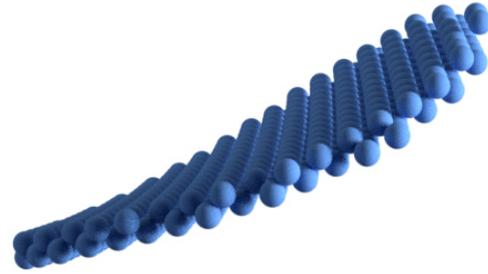
The frontiers and the challenges

Materials simulations have become a dominant force in the world of science and technology. The intellectual challenges lying ahead to sustain such a paradigm shift are discussed.

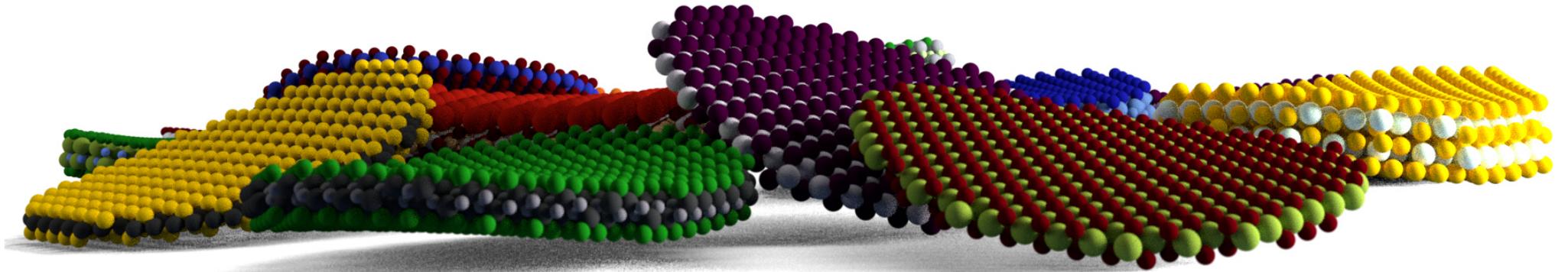
Nicola Marzari

- 1) PREDICTIVE ACCURACY**
- 2) REALISTIC COMPLEXITY**
- 3) MATERIALS' INFORMATICS**

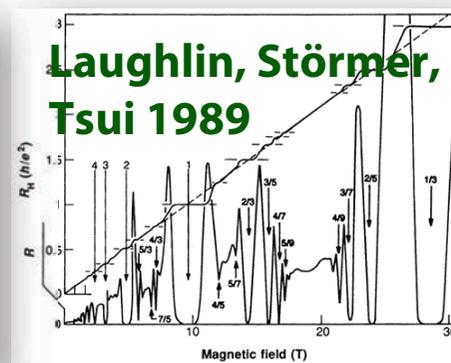




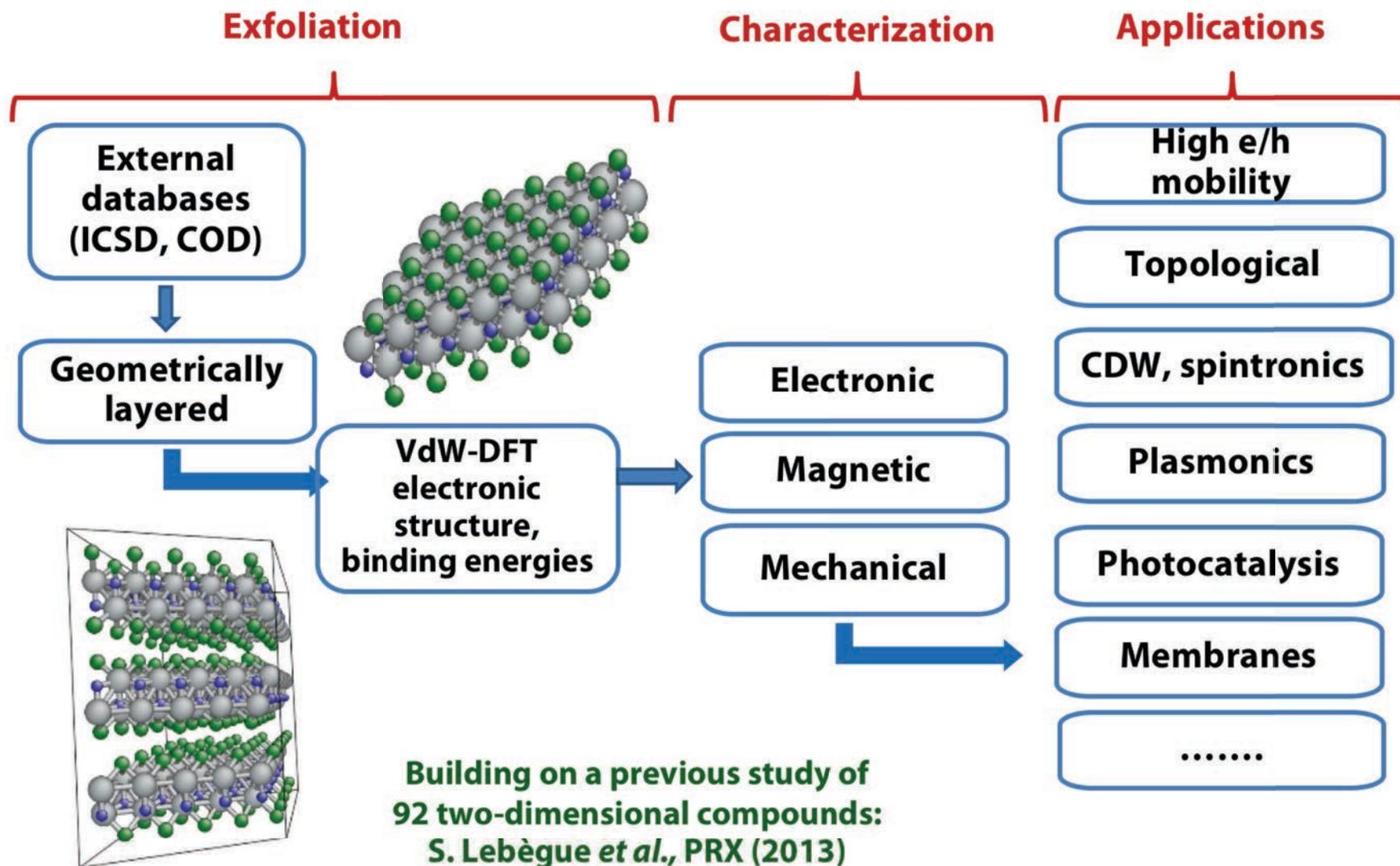
COMPUTATIONAL EXFOLIATION OF ALL KNOWN INORGANIC MATERIALS



PHYSICS AND CHEMISTRY IN LOW DIMENSIONS

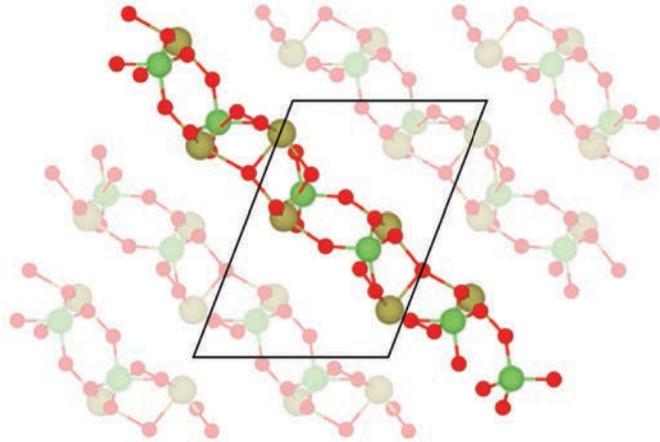


HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION

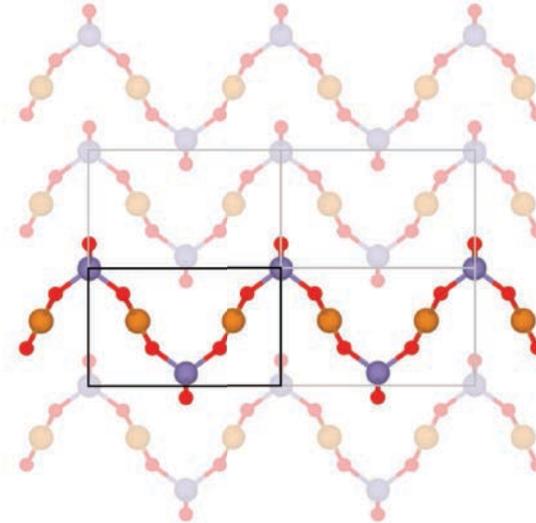


GEOMETRIC IDENTIFICATION OF LAYERED MATERIALS

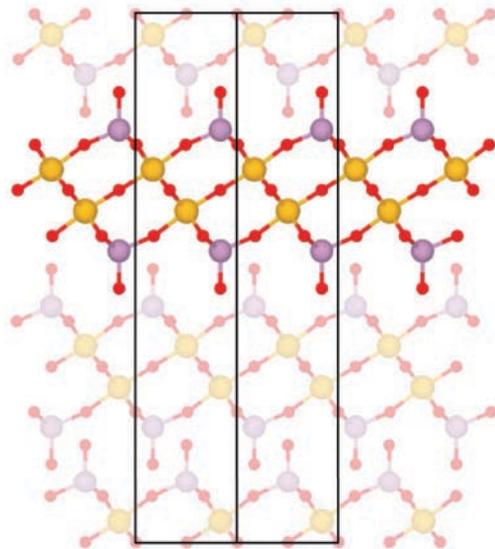
a



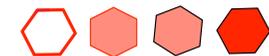
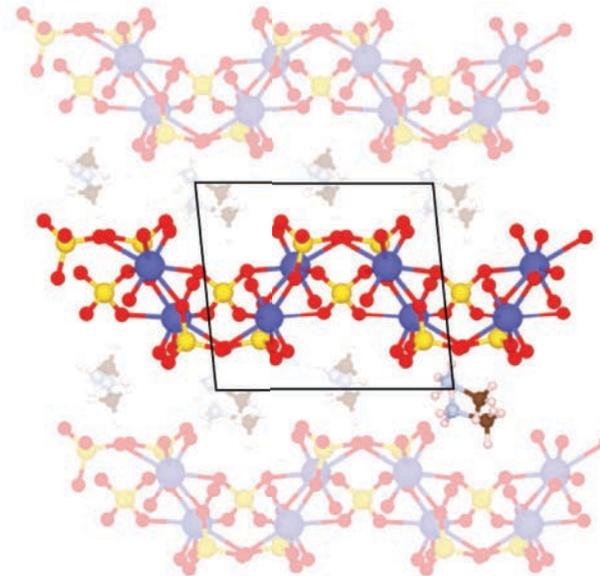
b



c



d



Automation

Automation
Remote management
High-throughput

Data

Database
Provenance
Storage

Environment

Research environment
Scientific workflows
Data analytics

Sharing

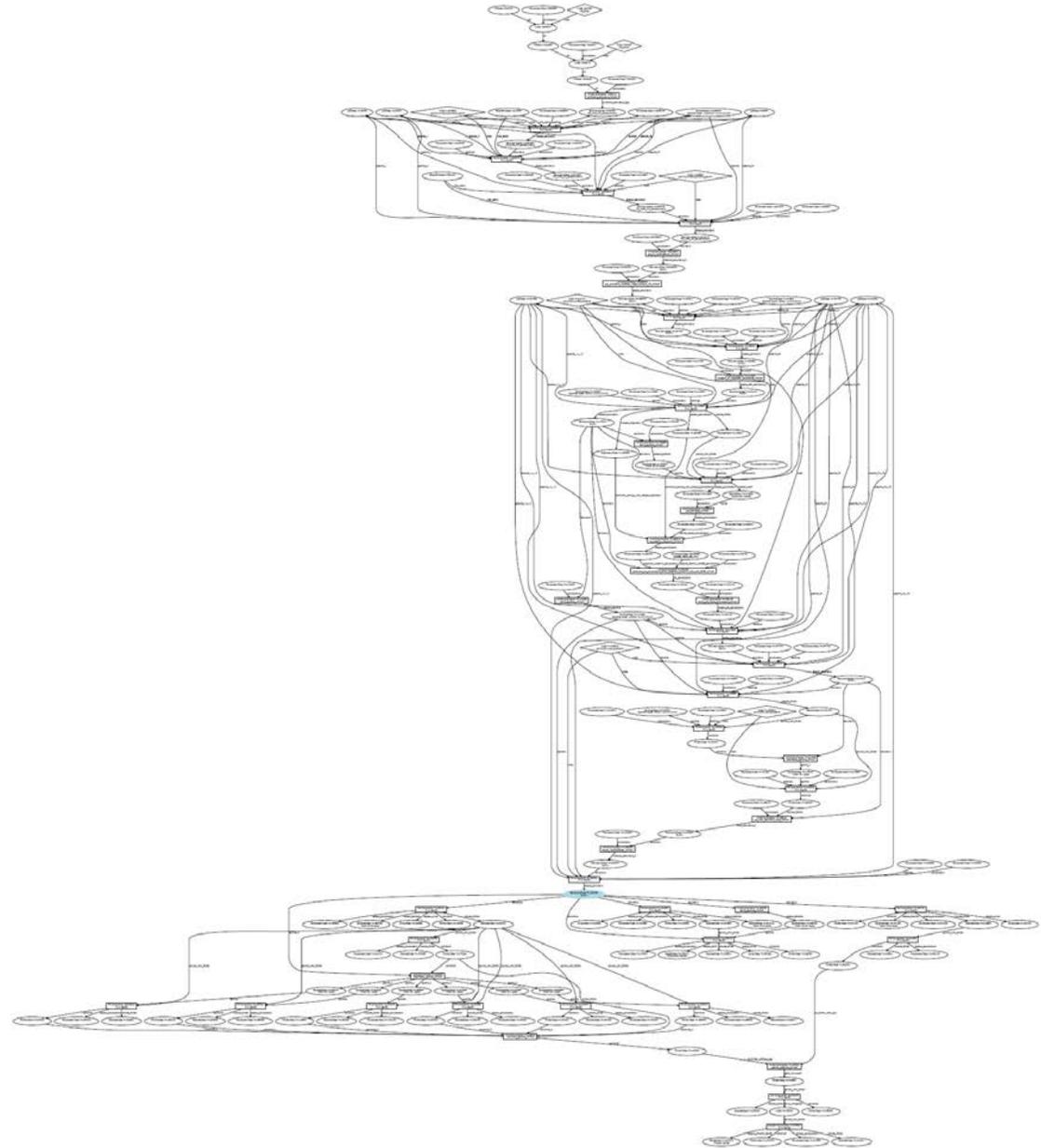
Social
Sharing
Standards



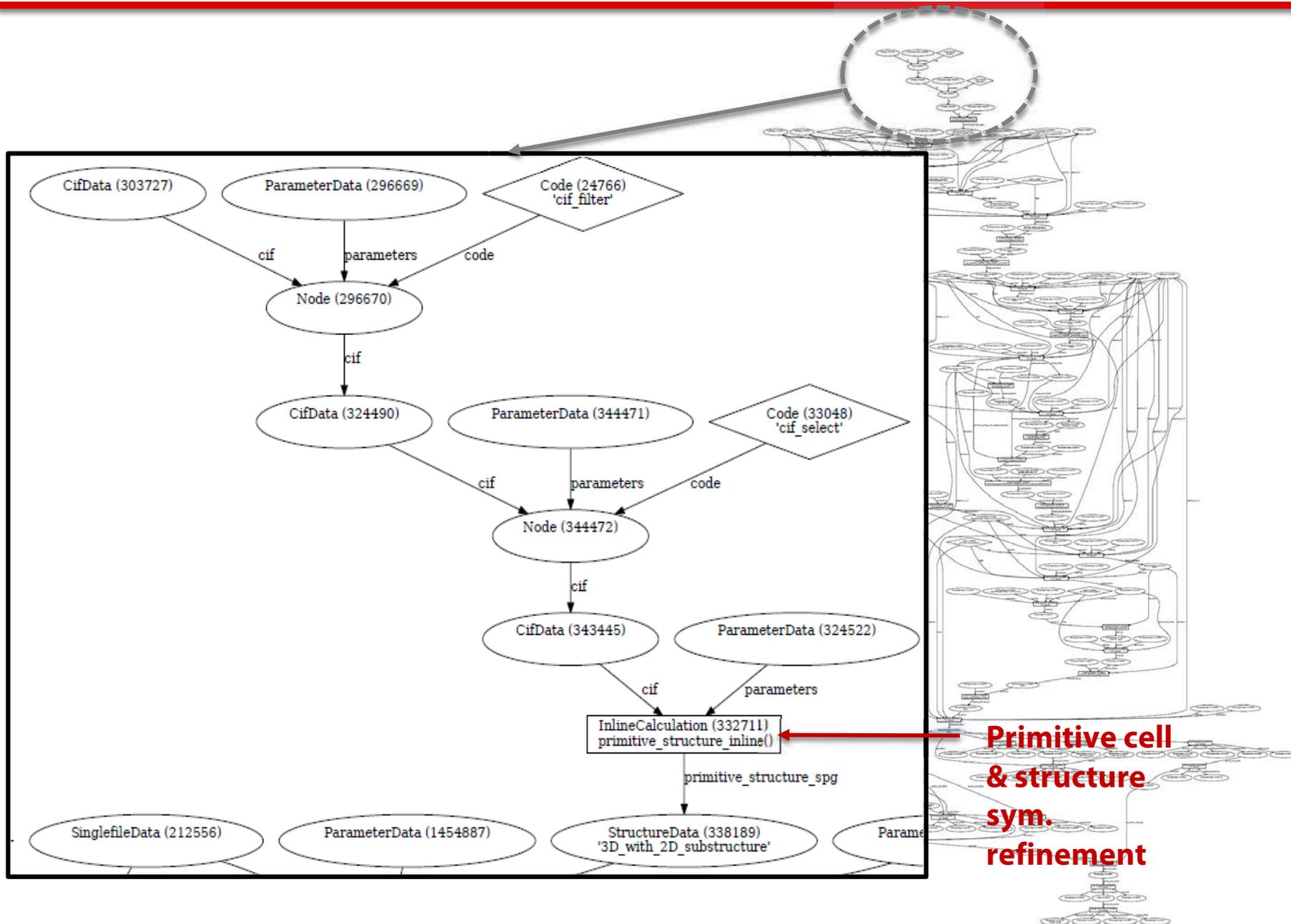
<http://www.aiida.net>

G. Pizzi et al., *Comp. Mat. Sci.* 111, 218 (2016)

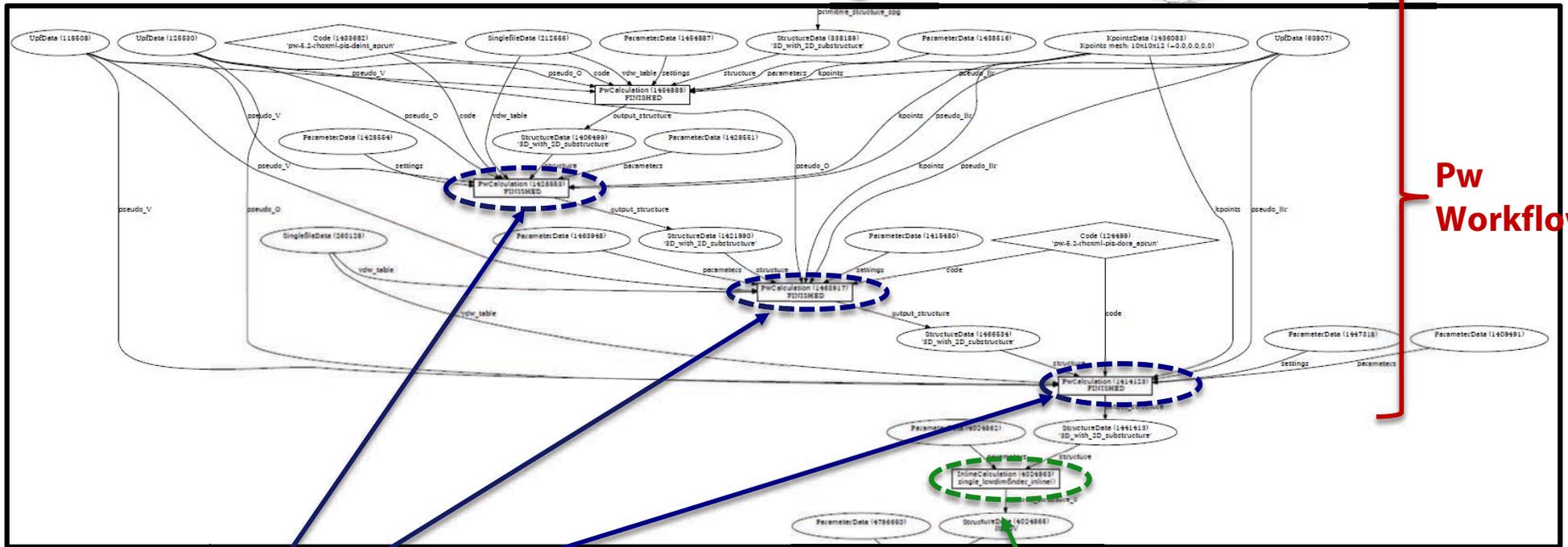
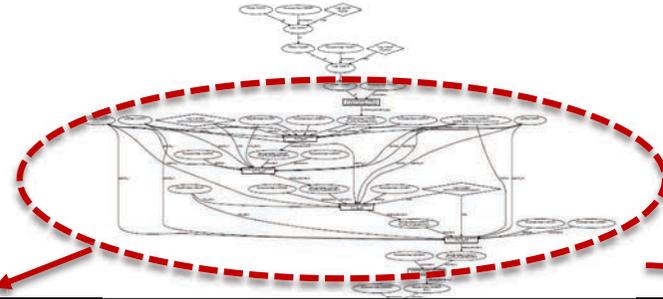
LET'S START WITH VOBr_2



FROM ICSD TO A WORKING STRUCTURE

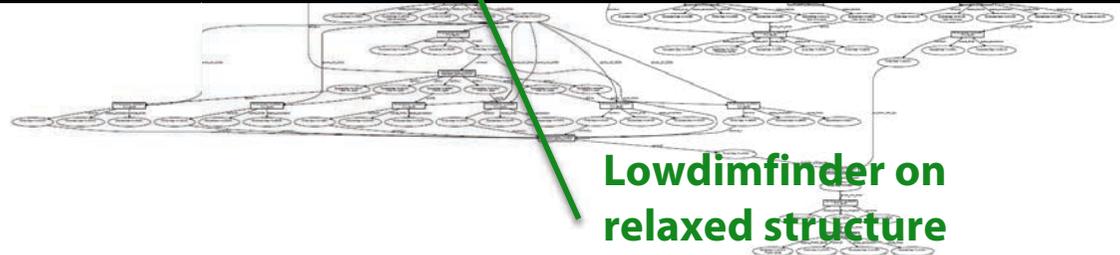


3D RELAXATION



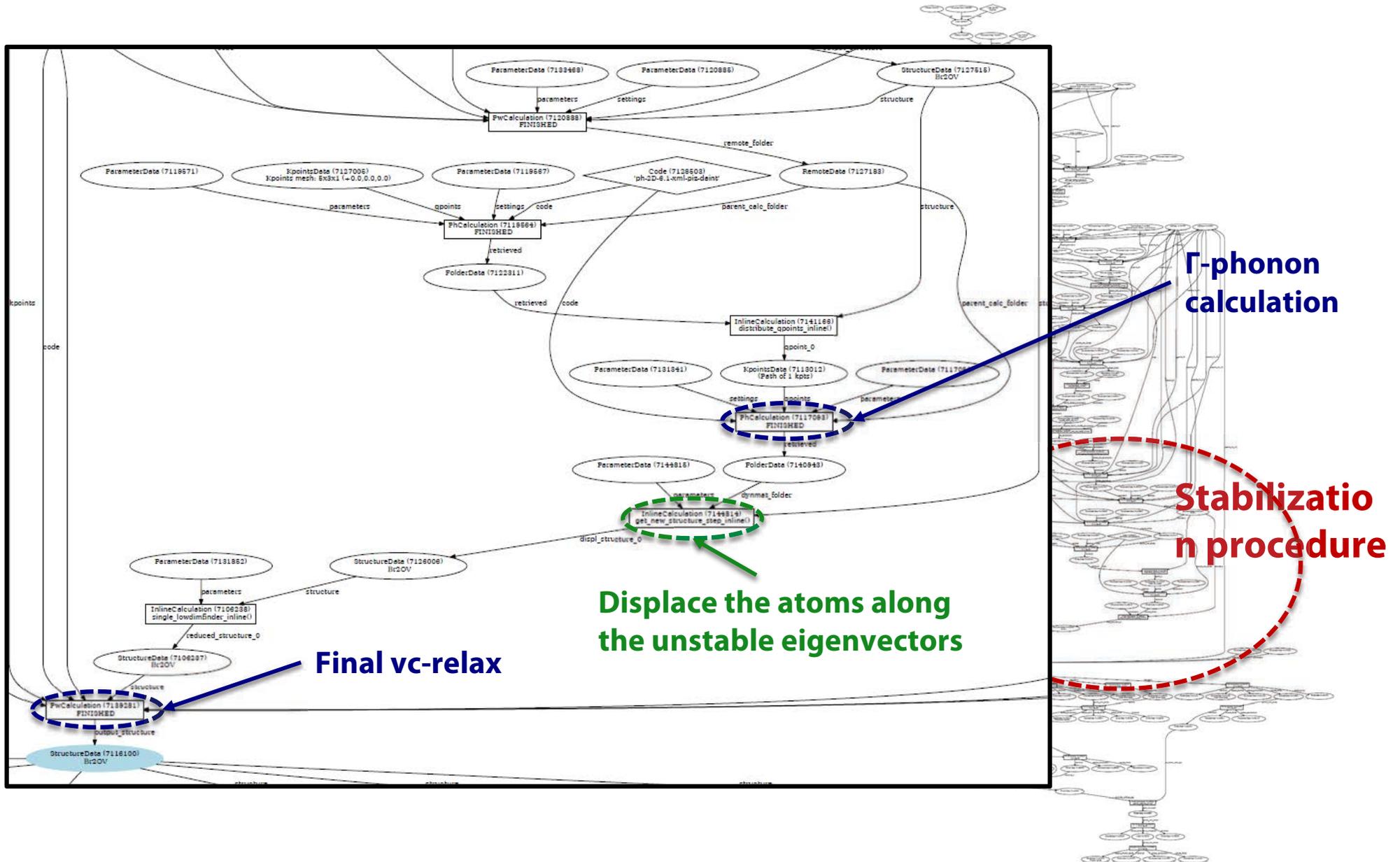
**Pw
Workflow**

Pw calculations



**Lowdimfinder on
relaxed structure**

REMOVING MECHANICAL INSTABILITIES



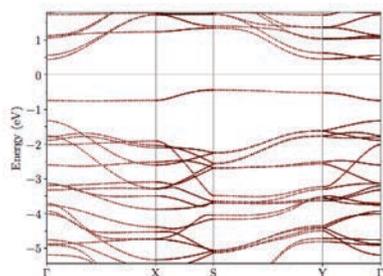
FINALLY...

215 VBr₂O (Pmm2)

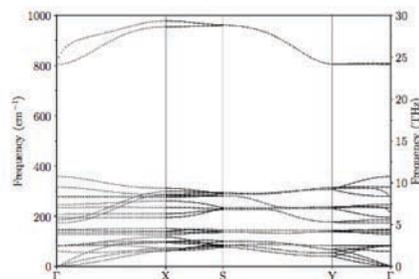
Info and properties (for more details and definitions see page 2)

Formula	VBr ₂ O	DF2-C09 Binding energy [meV/Å ²]	14.4
Spacegroup	Pmm2	rVV10 Binding energy [meV/Å ²]	21.6
Prototype	VCl ₂ O (Pmm2)	Band gap [eV]	0.9
Parent 3D	VBr ₂ O	Magnetic State	AFM
Source DB	ICSD	Tot. Magnetization [μ_B /cell]	0.0
DB ID	24381	Abs. Magnetization [μ_B /cell]	2.54

Band structure and phonon dispersions



Band structure: energy bands of VBr₂O (66 electrons) in a window around the chemical potential and along a high-symmetry path. The number of bands included in the calculation is 80.



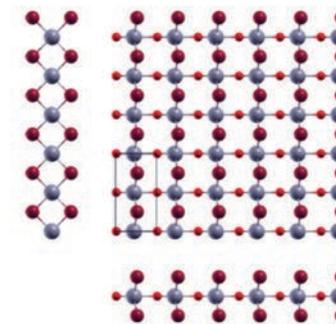
Phonon dispersions: phonon frequencies of VBr₂O (8 atoms/cell) along a high-symmetry path.

Crystal structure

Structural parameters: cell (top) and atomic positions (bottom) of VBr₂O in cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a_1	3.80622044	0.00000000	0.00000000
a_2	0.00000000	7.17029927	0.00000000
a_3	0.00000000	0.00000000	19.47346306

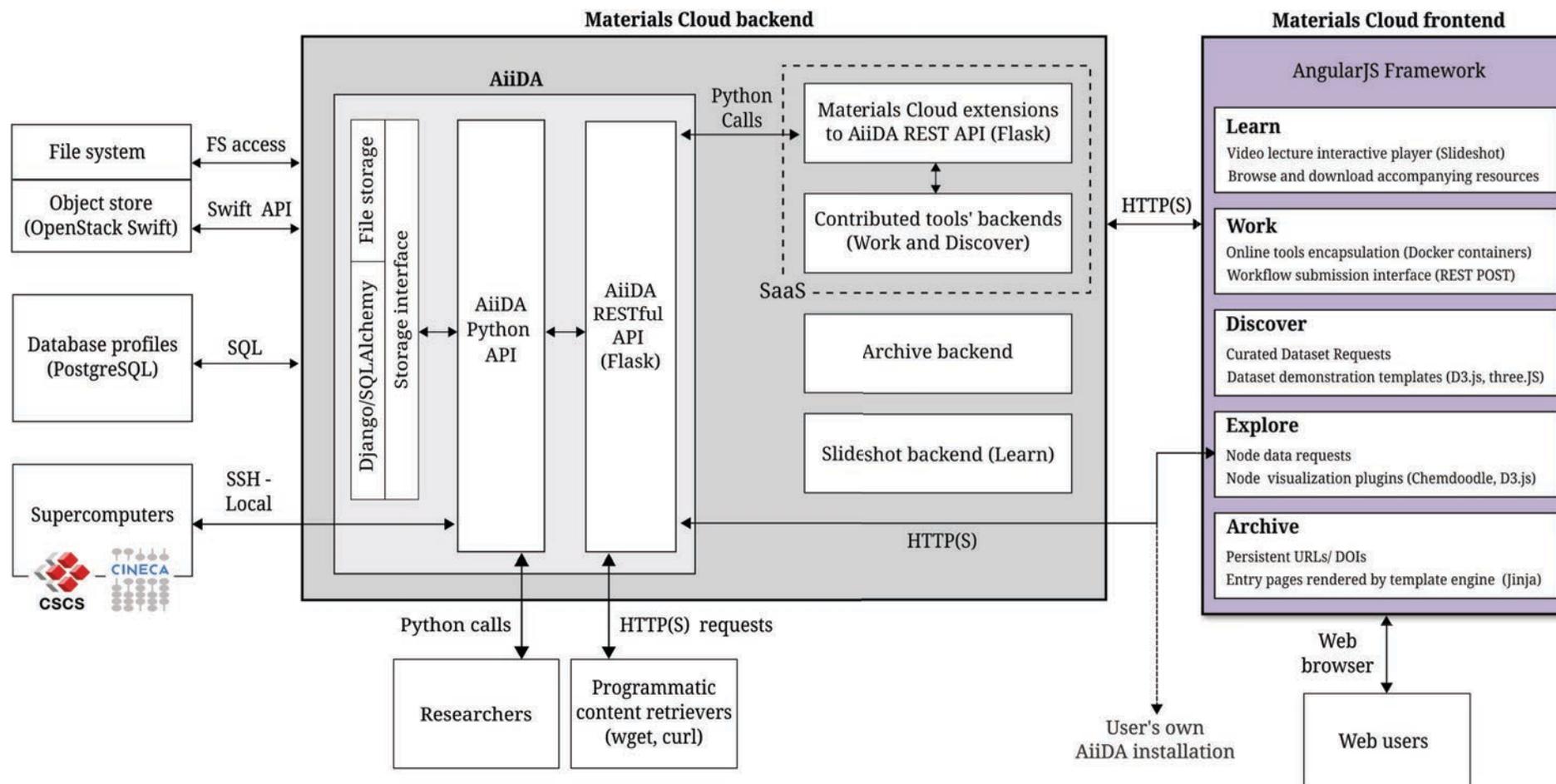
	x [Å]	y [Å]	z [Å]
• Br	2.00107500	5.37772439	-1.78545446
• Br	2.00107500	1.79257489	-1.78545446
• V ₁	1.70214333	3.58514964	0.00000000
• V ₂	1.70214341	0.00000000	0.00000000
• Br	2.00107500	5.37772439	1.78545446
• Br	2.00107500	1.79257489	1.78545446
• O ₁	0.06788642	3.58514964	0.00000000
• O ₂	0.06788661	0.00000000	0.00000000



Orthographic projections: different views of VBr₂O from the x axis (left), the y axis (bottom) and the z axis (center).



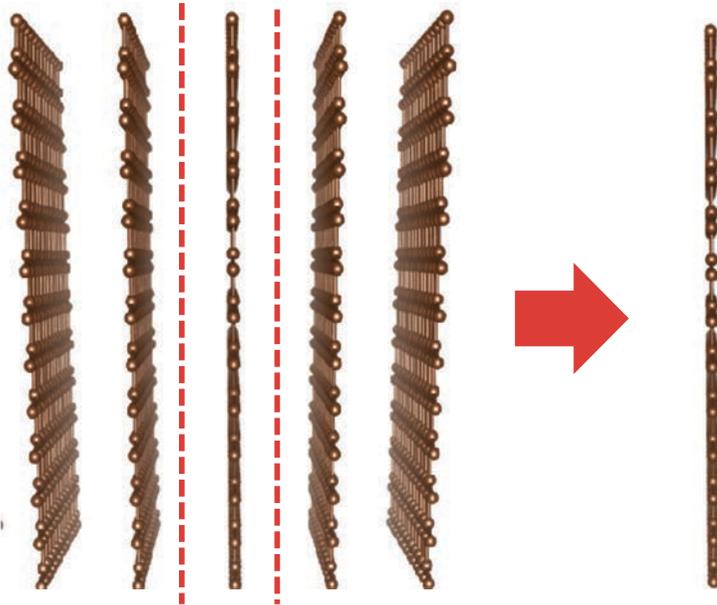
DISSEMINATION VIA THE MATERIALS CLOUD



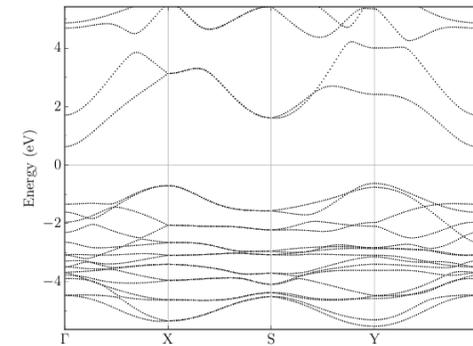
<http://www.materialscloud.org>



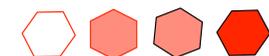
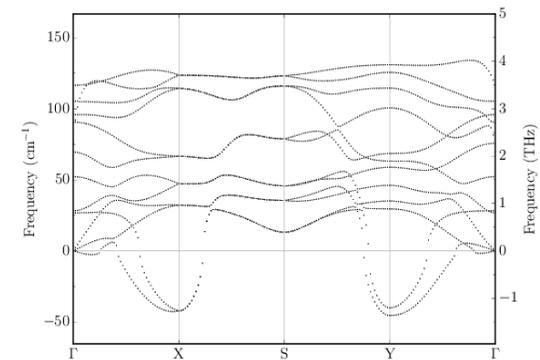
STABILITY ANALYSIS: MAGNETIC AND MECHANICAL



Band structures



Phonon dispersions



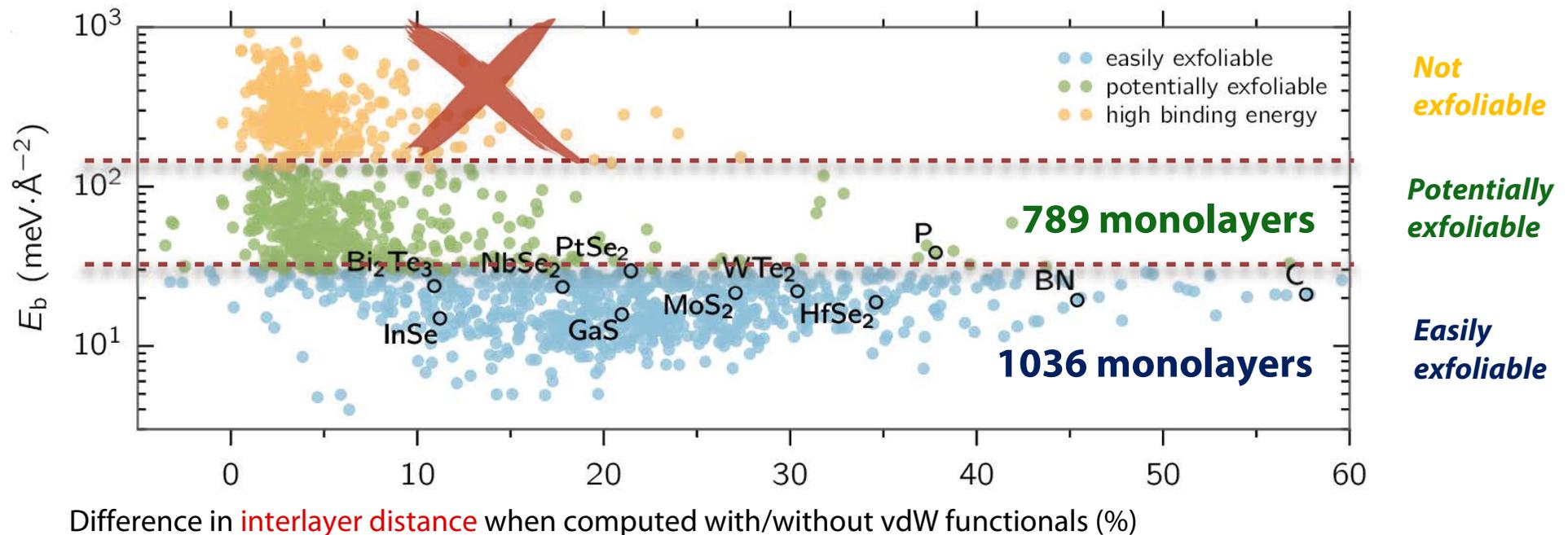
HOW MANY CANDIDATES? GEOMETRIC SCREENING

	Unique to COD	Unique to ICSD	Common to both	Total
Entries analyzed	307616	172370		479986*
CIF inputs	99212	87070		186282*
Unique 3D structures	60354	34548	13521	108423
Layered 3D structures	1180	3257	1182	5619

*At this level unicity is not tested



HOW MANY CANDIDATES? GEOMETRIC SCREENING

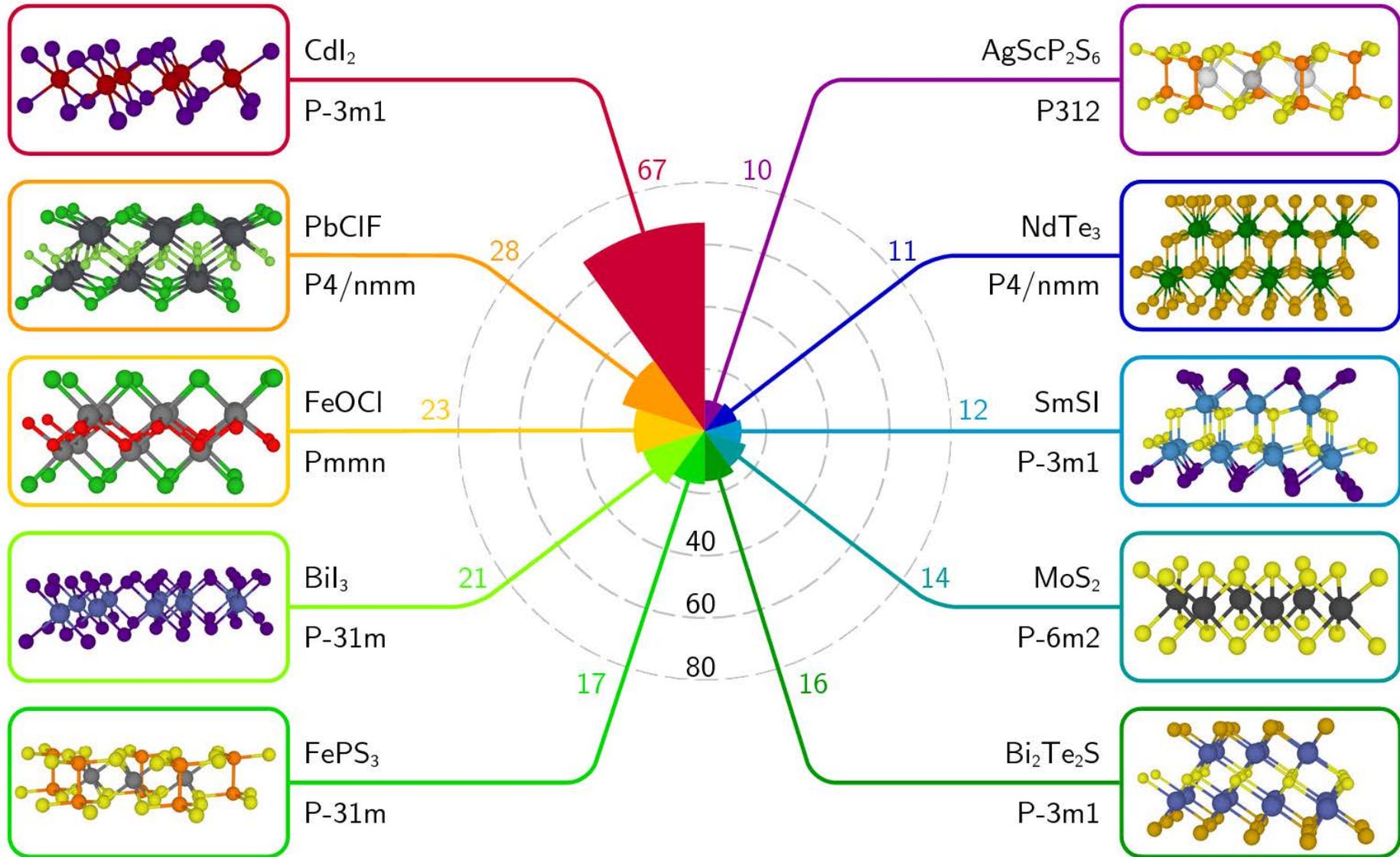


- $E_b < 30 \text{ meV}/\text{\AA}^2$ (DF2-C09) or $E_b < 35 \text{ meV}/\text{\AA}^2$ (rVV10) \rightarrow 2D, easily exfoliable
- In-between \rightarrow 2D, potentially exfoliable
- $E_b > 130 \text{ meV}/\text{\AA}^2 \rightarrow$ not 2D (discarded)

<https://www.materialscloud.org/discover/2dstructures>



2D PROTOTYPES



JACUTINGAITE (Pt_2HgSe_3)

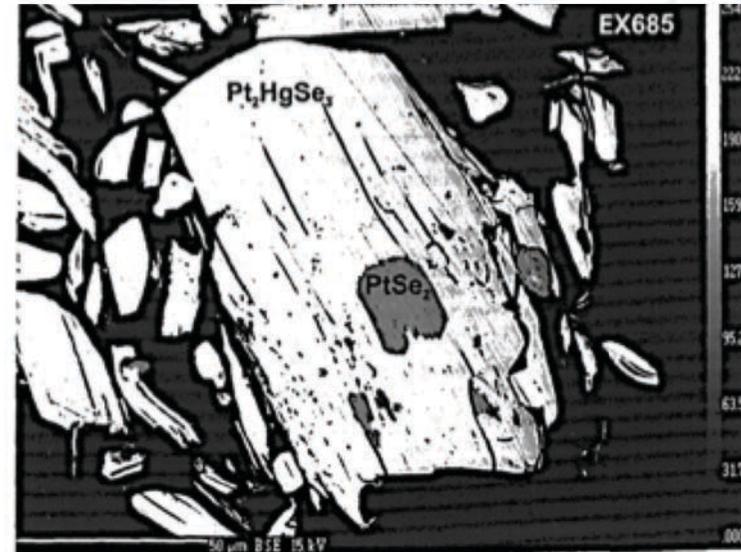
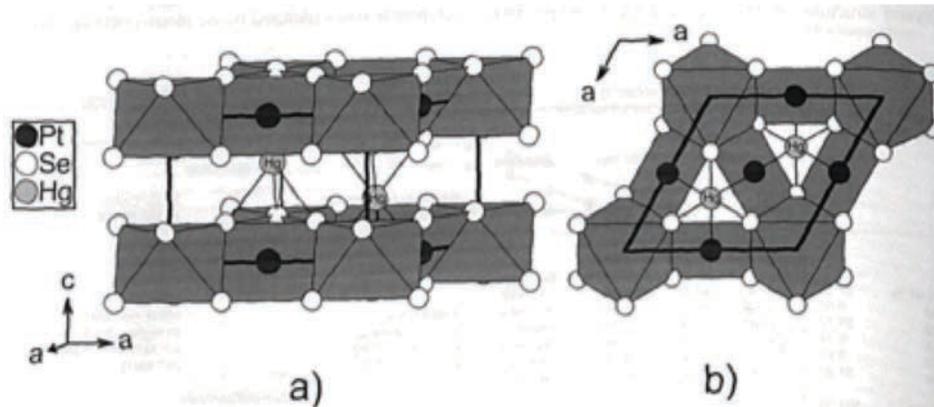
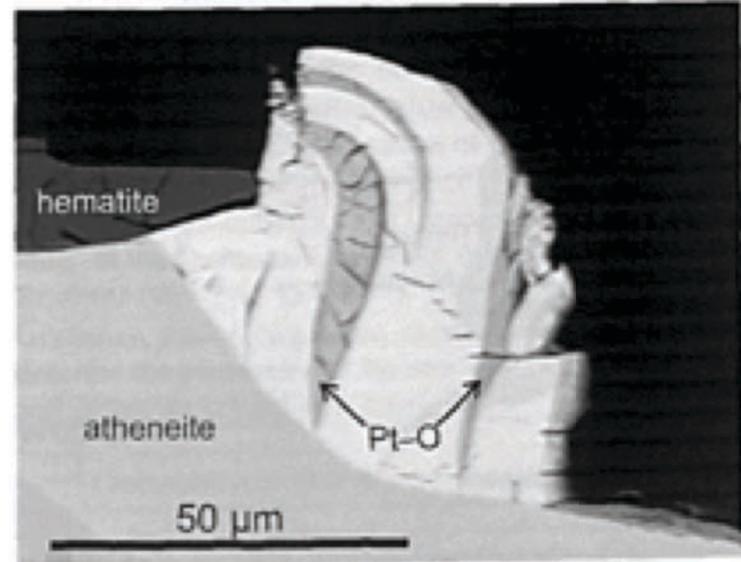
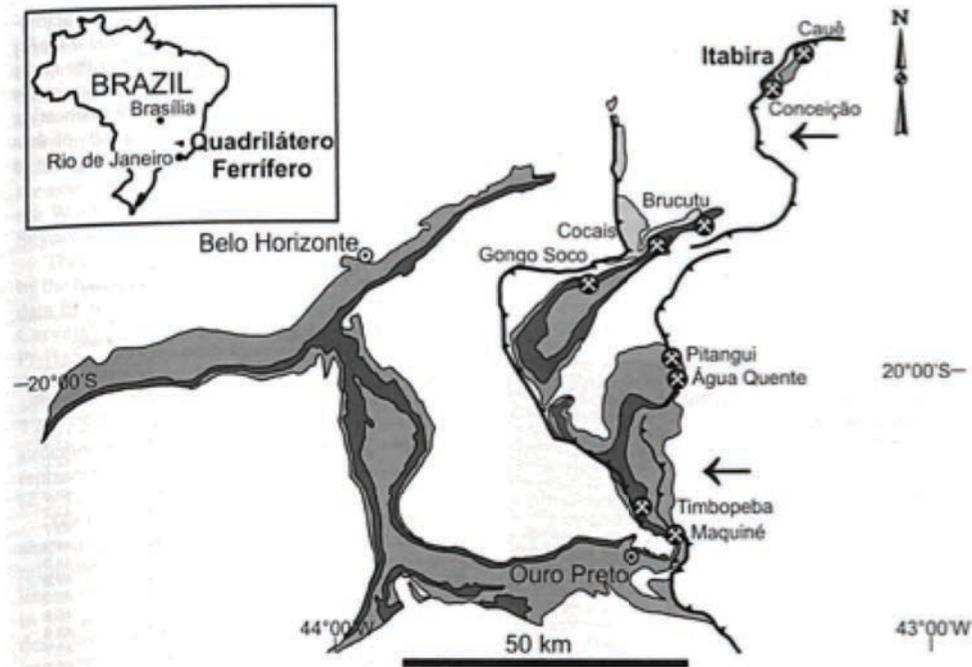
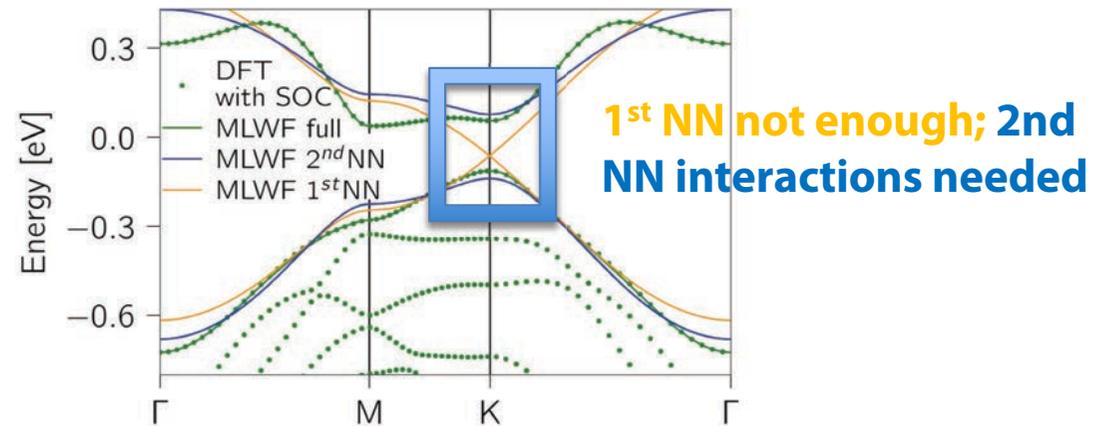
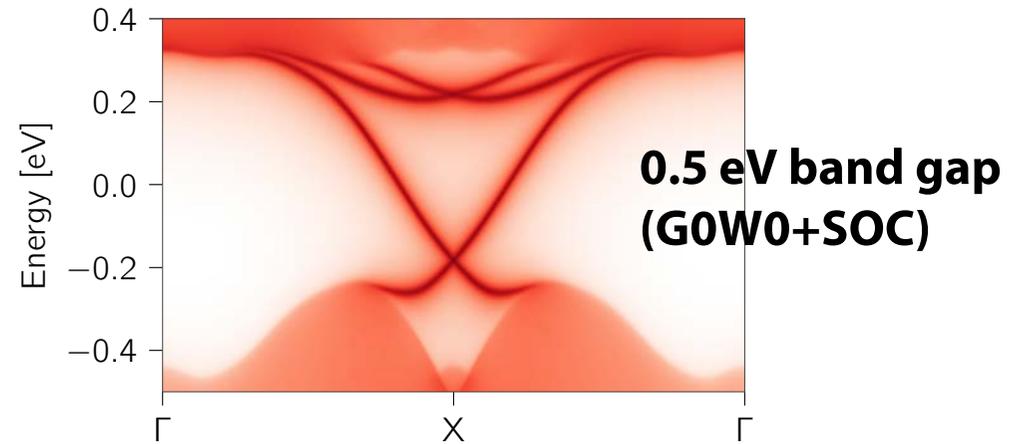
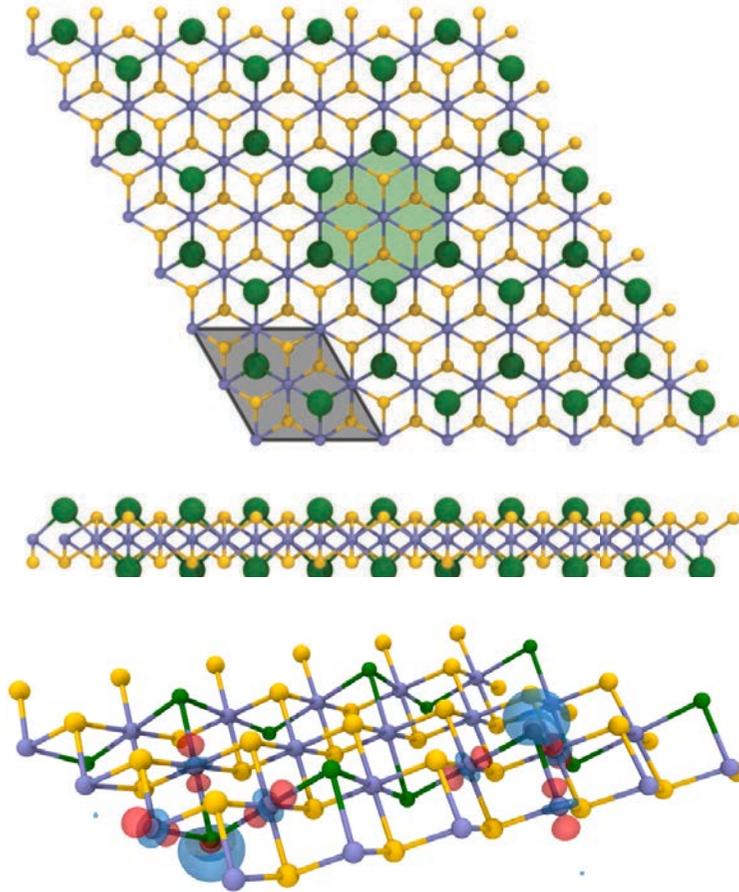


FIG. 3. Back-scattered electron microphotograph of Pt_2HgSe_3 (light) and PtSe_2 (dark inclusions) grown at 400°C (run EX685). Scale bar (50 μm) appears at lower left.

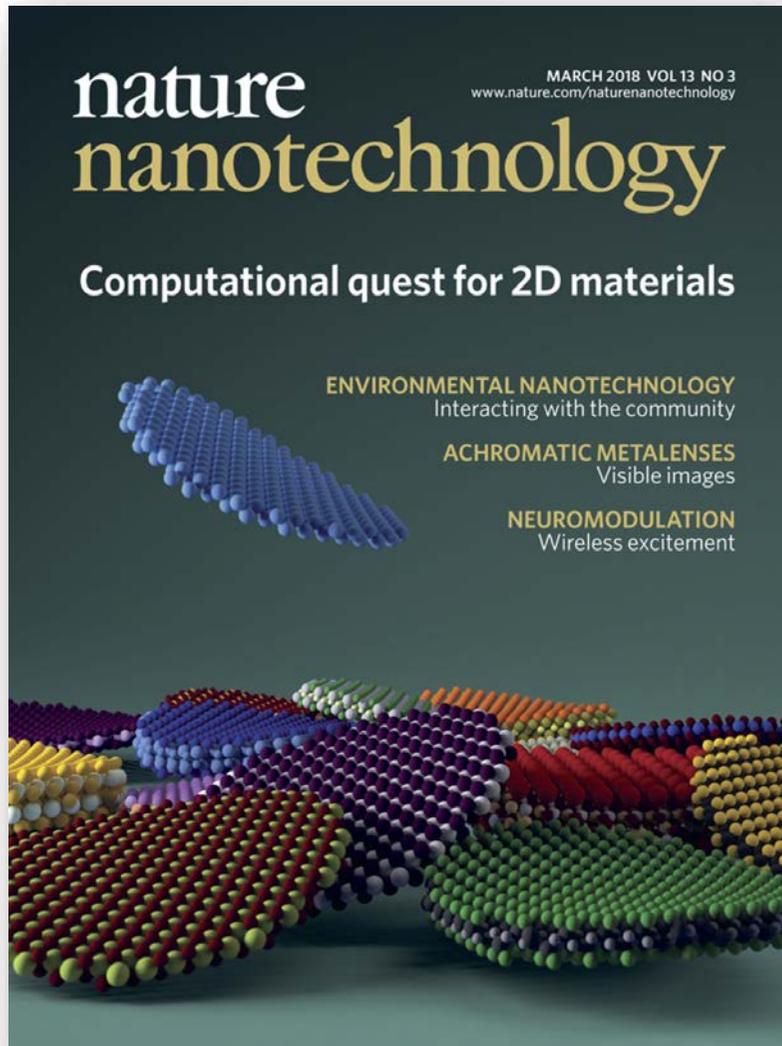
MONOLAYER JACUTINGAITE AS A KANE-MELE QSHI



A. Marrazzo *et al.*, Phys. Rev. Lett. 120 117701 (2018)



THERE IS PLENTY OF ROOM AT THE TOP



**N. Mounet et al., Nature Nanotechnology
13, 246 (2018)**

2D children:

- **High electron/hole mobility devices**
- **Topological insulators, quantum computing**
- **Ferromagnetic/spintronics in 2D**
- **Charge-density waves and superconductors**
- **Plasmonics, transparent conductors**

3D layered parents:

- **Solid-state ionic conductors**
- **Hydrogen or oxygen evolution catalysts**
- **Membranes for filtration/separation**
- **Piezo, ferro, and thermoelectrics**

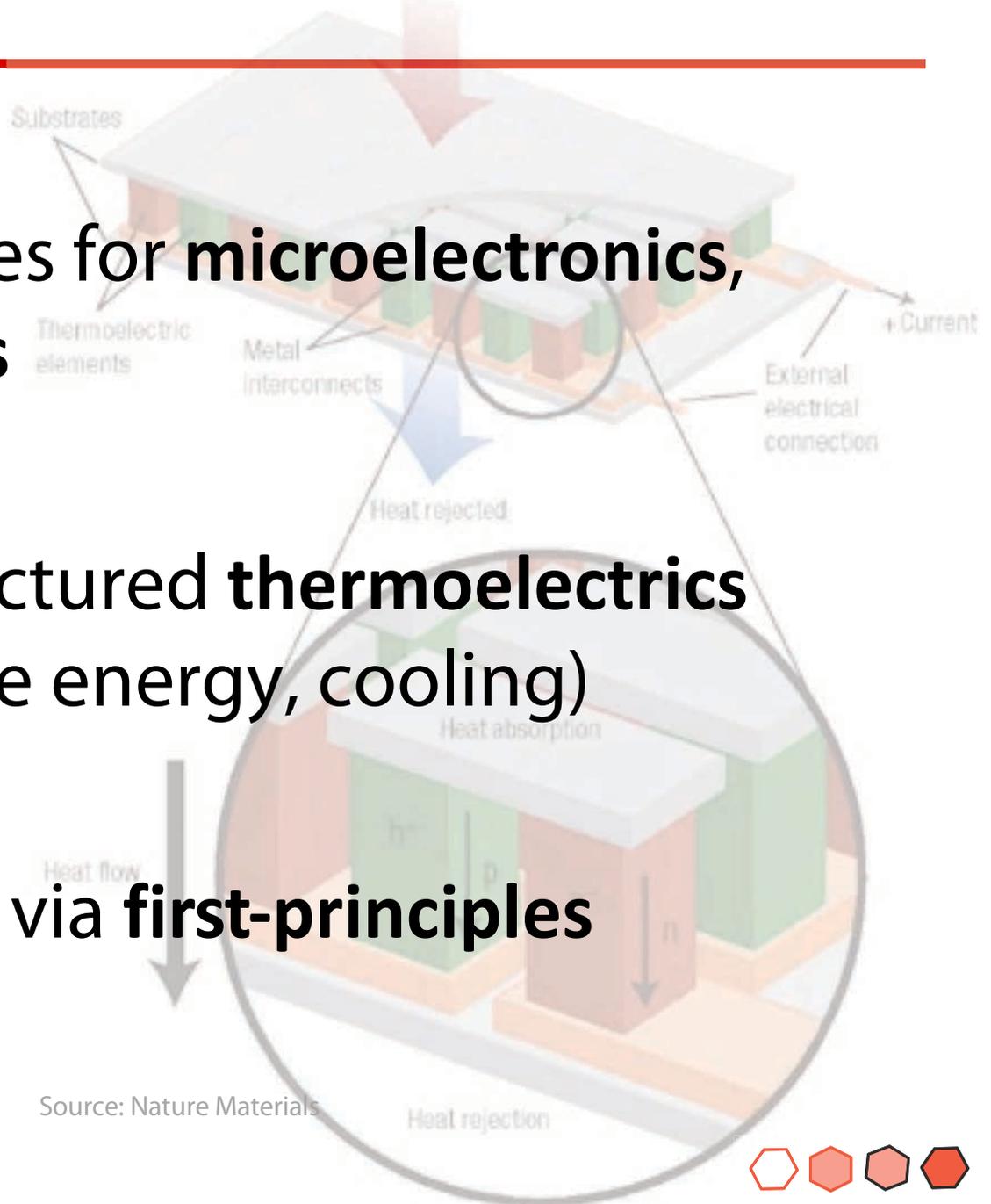
COMPLEXITY

- **From total energy to thermodynamics**
 - temperature, pressure, chemical potentials and partial pressures, electrochemical potential, pH
- **Length, time, phase and composition sampling**
 - linear scaling, multiscale,
 - metadynamics, sketch-map
 - minima hopping, random-structure searches
- **Complex properties**
 - spectroscopies and microscopies: IR, Raman, XPS, XANES, NMR, EPR, ARPES, STM, TEM...
 - composition-temperature phase diagrams
 - electronic and thermal transport: ballistic, Keldysh, Boltzmann
 - electron-hole interactions



MULTISCALE TRANSPORT

- Nanoscale devices for **microelectronics, quantum devices**
- Bulk or nanostructured **thermoelectrics** (harvesting waste energy, cooling)
- Characterization via **first-principles spectroscopies**



ELECTRICAL RESISTIVITY (TEMP, DOPING)

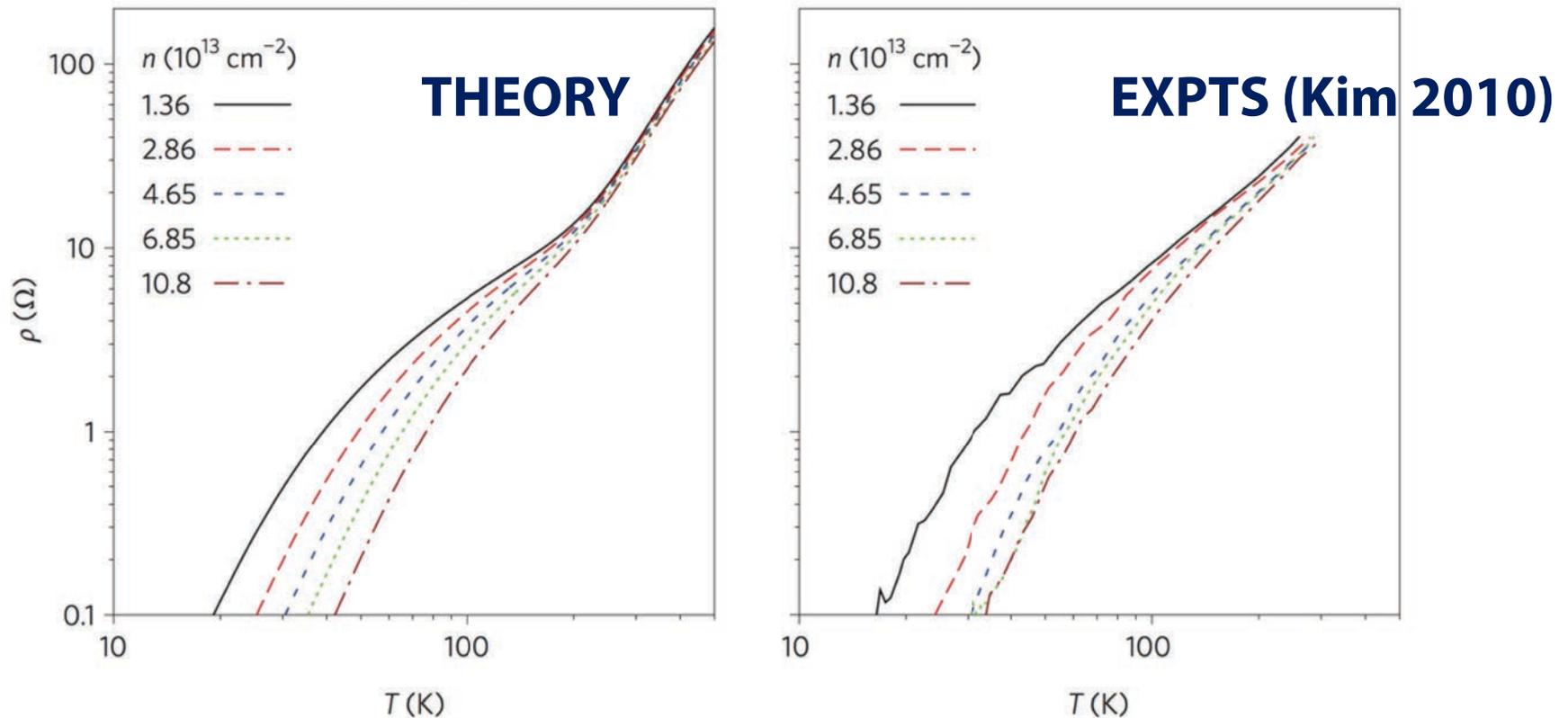


Figure 1 | Electrical resistivity of graphene as a function of temperature and doping (ρ , electrical resistivity; T , temperature; n , carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation theory and Wannier interpolations to solve the Boltzmann transport equation. Right panel: experimental data. Adapted from ref. 4, American Chemical Society.

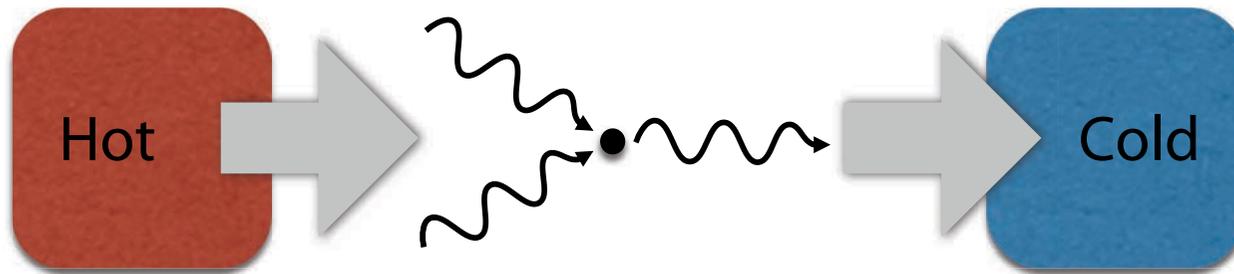
C.-H. Park *et al.*, Nano Letters (2014)

T. Y. Kim, C.-H. Park, and N. Marzari, Nano Letters (2016)



LINEARIZED BOLTZMANN EQUATION

Phonon population at equilibrium: $\bar{n}_\nu = \frac{1}{e^{\hbar\omega_\nu/k_B T} - 1}$ $\nu = (\mathbf{q}, s)$
 Phonon population at out-of-equilibrium conditions ∇T : index on all states



Boltzmann transport equation

$$\frac{\partial n_\nu(\vec{x}, t)}{\partial t} + \vec{v}_\nu \cdot \nabla n_\nu(\vec{x}, t) = - \sum_{\nu'} \Omega_{\nu\nu'} n_{\nu'}(\vec{x}, t)$$

Diffusion / Liouville

Collision / scattering

Heat flux: $Q = \frac{1}{V} \sum_{\nu} \hbar\omega_\nu v_\nu n_\nu$ operator (linearised)



RELAXATION-TIME APPROXIMATION

Often, the Boltzmann equation is simplified with the single-mode relaxation time approximation (SMA), i.e. retaining the diagonal part of the scattering matrix:

$$\frac{\partial n_\nu}{\partial t} + \cancel{v_\nu \cdot \nabla} n_\nu \approx -\frac{n_\nu}{\tau_\nu^{SMA}}$$

In a homogeneous system ($\nabla n_\nu=0$) the population n_ν decays to equilibrium with a relaxation time τ_ν^{SMA}



RELAXATION-TIME APPROXIMATION

Often, the Boltzmann equation is simplified with the single-mode relaxation time approximation (SMA), i.e. retaining the diagonal part of the scattering matrix:

$$\cancel{\frac{\partial n_\nu}{\partial t}} + v_\nu \cdot \nabla n_\nu \approx -\frac{n_\nu}{\tau_\nu^{SMA}}$$

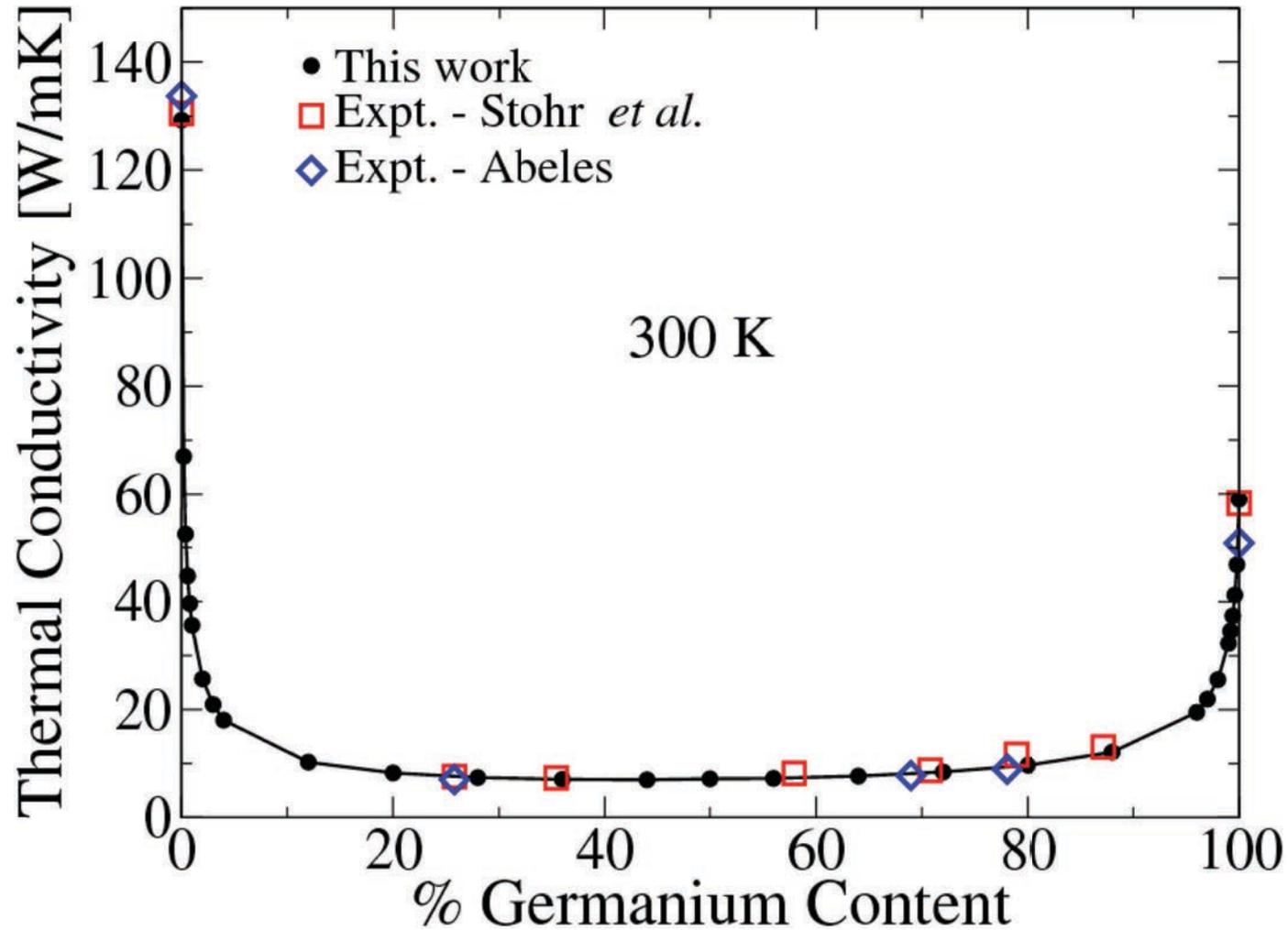
In a homogeneous system ($\nabla n_\nu = 0$) the population n_ν decays to equilibrium with a relaxation time τ_ν^{SMA}

At steady state $K \sim \sum_\nu C_\nu v_\nu \Lambda_\nu^{SMA}$

Kinetic theory; each scattering leads to thermalisation



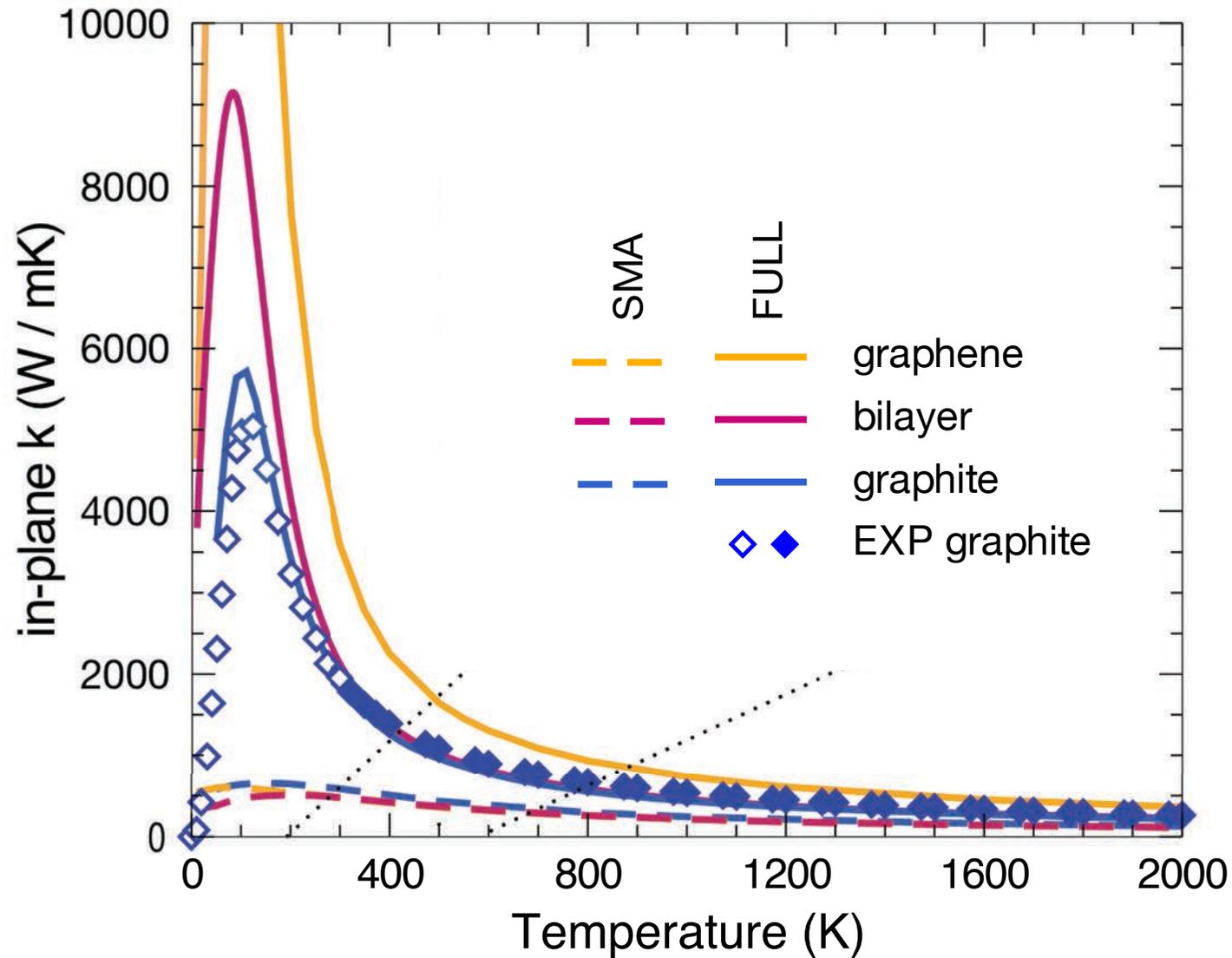
COMPOSITION DEPENDENCE IN $\text{Si}_{1-x}\text{Ge}_x$ ALLOYS



J. Garg, N. Bonini, B. Kozinsky and N. Marzari, *Phys. Rev. Lett.* (2011)



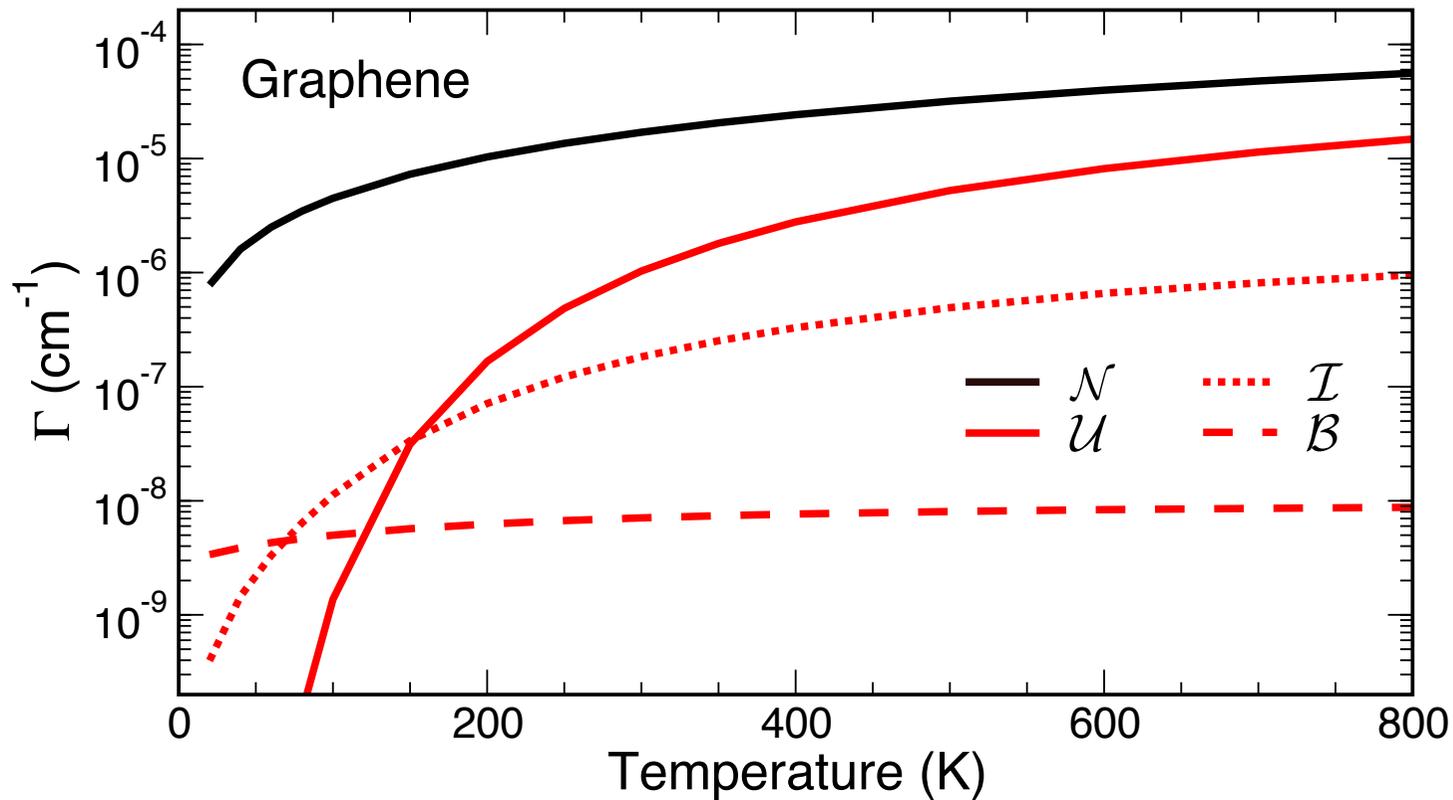
LAYERED MATERIALS



G. Fugallo, A. Cepellotti, et al. (Nano Letters, 2014)



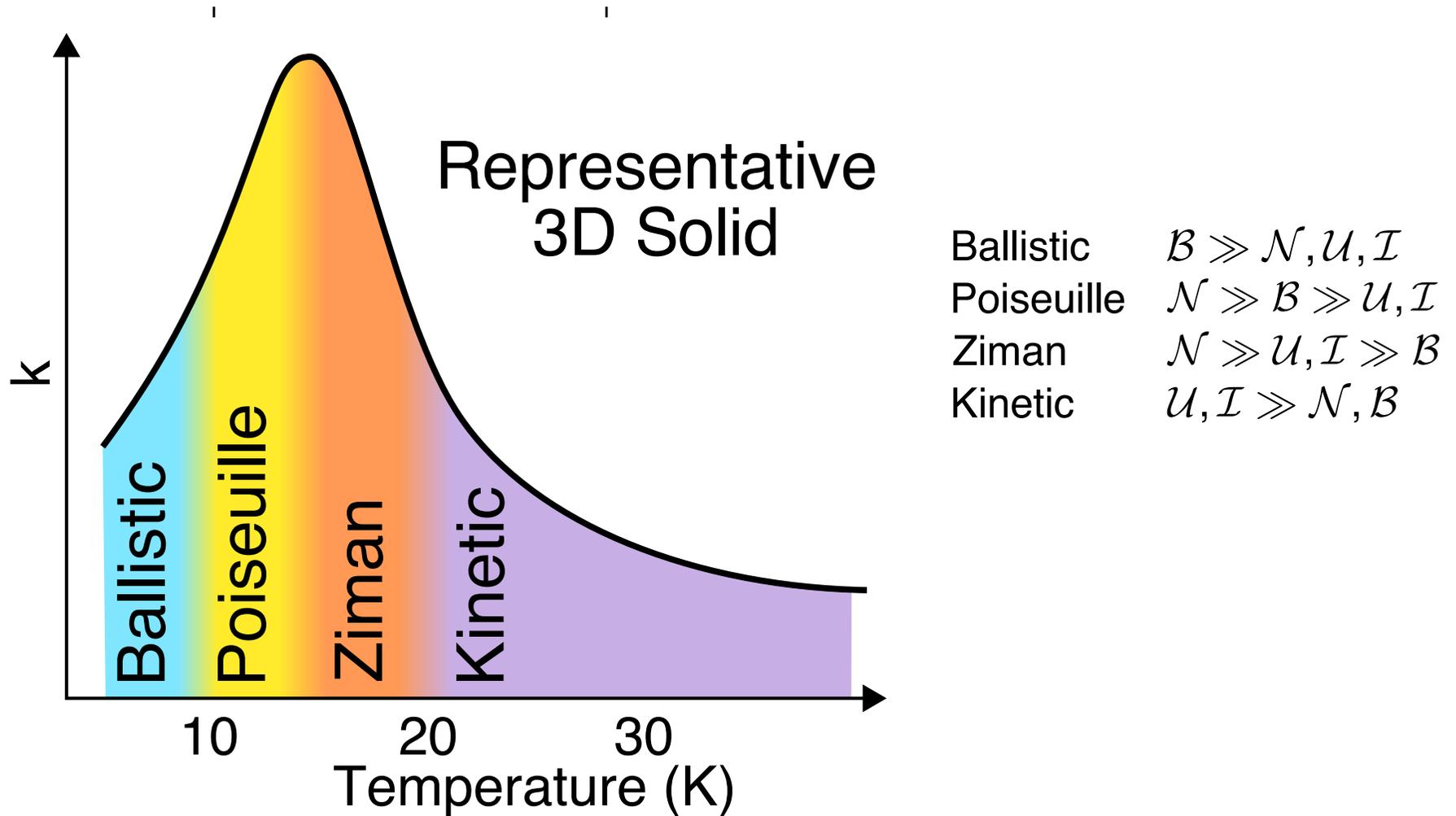
NORMAL PROCESSES DOMINATE



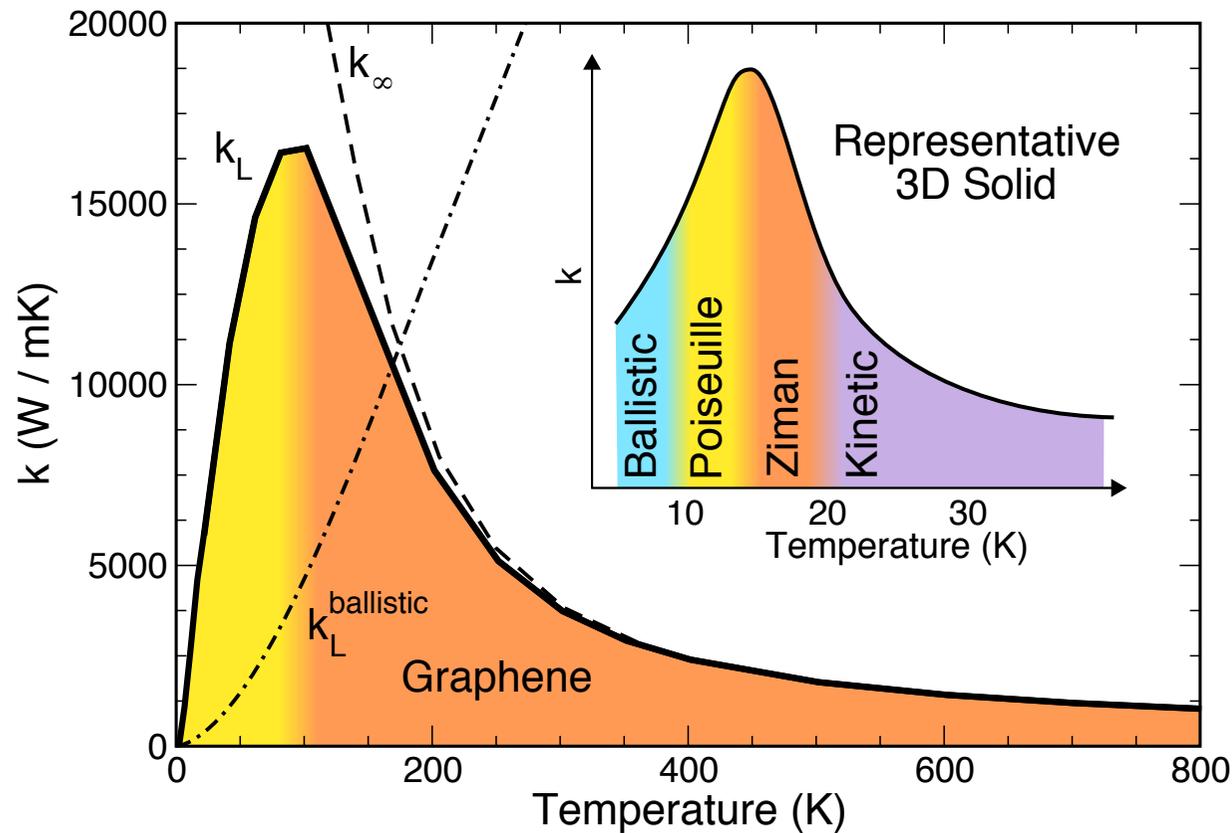
Linewidths for graphene, natural abundance, 100μ



POISEUILLE AND ZIMAN HYDRODYNAMICS



POISEUILLE AND ZIMAN HYDRODYNAMICS



Ballistic	$B \gg N, U, I$
Poiseuille	$N \gg B \gg U, I$
Ziman	$N \gg U, I \gg B$
Kinetic	$U, I \gg N, B$



BREAKDOWN OF THE PHONON PICTURE

- the time scale of phonon scattering (i.e. the phonon lifetime) differs from that of heat flux dissipation;
- phonons are not the heat carriers;
- how can we define heat carriers and relaxation times?

To define heat carriers, **we diagonalise the scattering operator:**

$$\frac{1}{\mathcal{V}} \sum_{\nu'} \tilde{\Omega}_{\nu\nu'} \theta_{\nu'}^{\alpha} = \frac{1}{\tau_{\alpha}} \theta_{\nu}^{\alpha}$$



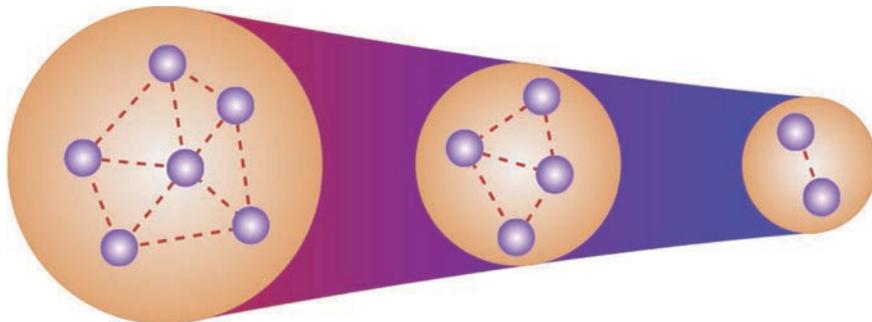
FROM PHONONS TO RELAXONS

Express the Boltzmann equation in the new basis (f_α is now the population of relaxon α):

$$\frac{\partial f_\alpha(\vec{X}, t)}{\partial t} + \sum_{\beta} \vec{V}_{\alpha\beta} \cdot \nabla f_\beta(\vec{X}, t) = -\frac{1}{\tau_\alpha} f_\alpha(\vec{X}, t)$$

The rotated equation now is diagonal in the scattering part; we can extract time scales for heat flux dissipation!

So, rather than phonons, we study the collision eigenvectors, that we will call **relaxons**.



A. Cepellotti and N. Marzari, PRX (2016);
Viewpoint on
<https://physics.aps.org/articles/v9/118>

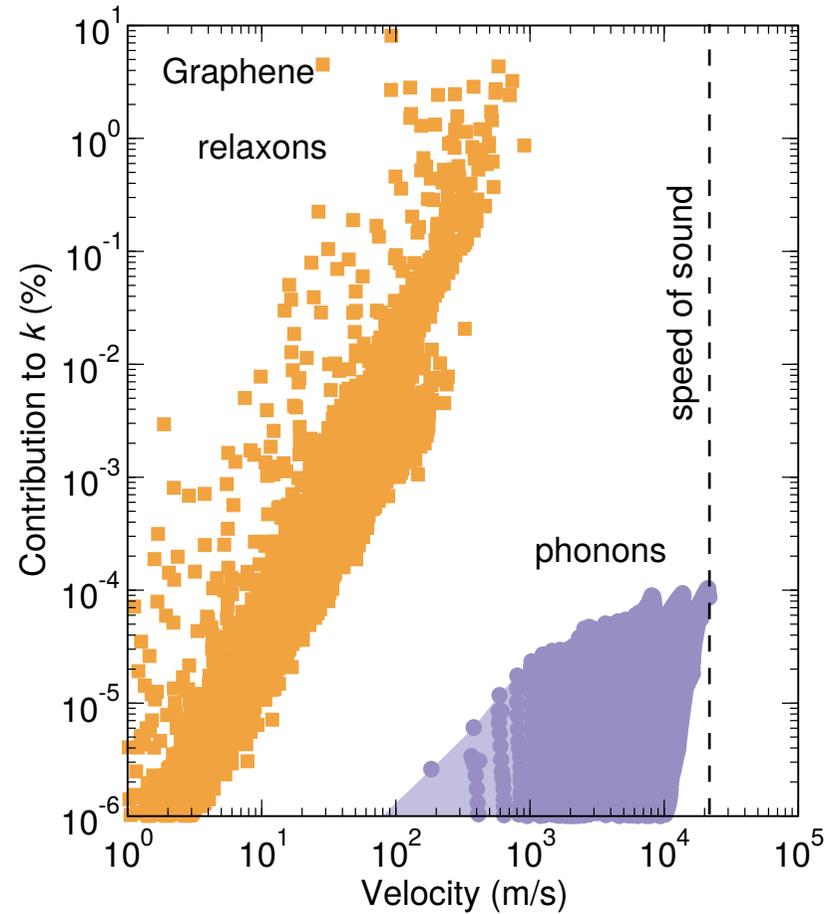


SUMMARY

	Phonon	Relaxon
Definition	Eigenstate of harmonic Hamiltonian	Eigenstate of collision matrix
Physical meaning	Collective excitation of atomic displacements Quantum of vibrational energy	Collective excitation of phonon populations Elementary carrier of heat
Exact quantities	Lifetime, velocity and mean free path of the vibration Quasiparticle (energy, wavevector, dispersion relations)	Relaxation time, velocity and mean free path of the heat carrier No dispersion relations
Thermal conductivity	Only obtained as solution of the BTE	Obtained as a kinetic theory of the relaxon gas



VELOCITY SCALE



**A. Cepellotti and N. Marzari, PRX (2016),
J. Hua, G. Vanacore, A. Cepellotti, N. Marzari, and A. H. Zewail, PNAS (2016)**



TRANSPORT WAVES IN THE LBTE

- Search for a wave solution for the phonon excitation numbers

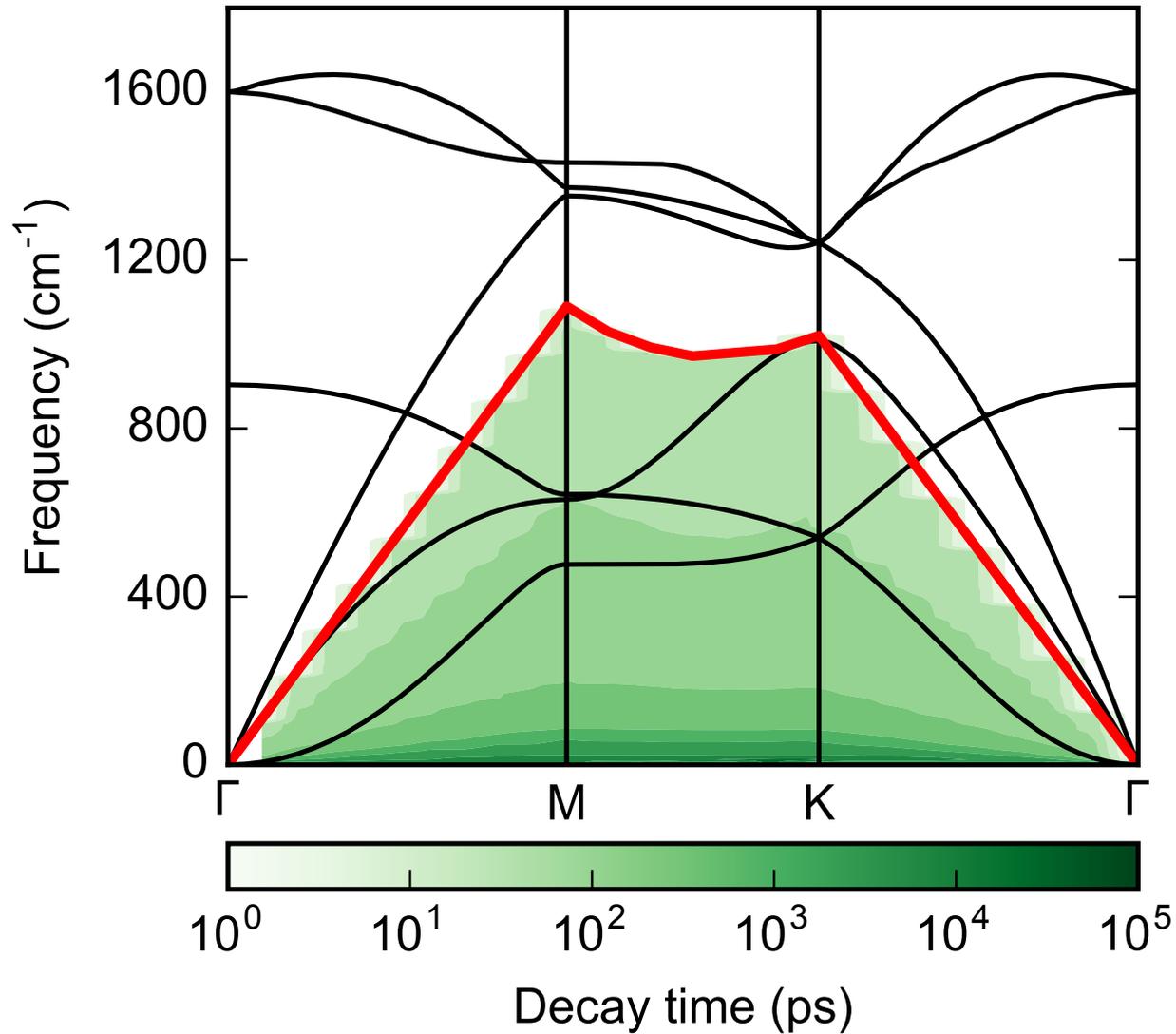
$$\Delta n_{\mu} = \Re \left(I_{\mu} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \right)$$

- i.e. Laplace transform the LBTE

$$-i\omega I_{\mu} + iI_{\mu} \mathbf{k} \cdot \mathbf{v}_{\mu} + \frac{1}{\mathcal{V}} \sum_{\mu'} \Omega_{\mu\mu'} I_{\mu'} = 0$$



TRANSPORT WAVES IN THE LBTE



A. Cepellotti and N. Marzari, PR Materials (2017)



TRANSPORT CONCLUSIONS

1. Thermal transport can be described accurately from first-principles
2. In layered or 2D materials the phonon picture breaks down, and **hydrodynamic phenomena**/collective excitations emerge
3. **Relaxons** as the individual carriers of heat
4. Surface scattering as a **friction effect**
5. **Transport waves** solutions for the LBTE – generalization of second sound



THERMAL THANKS



Andrea Cepellotti
(Berkeley)

2017 EPFL IBM PRIZE

2018 APS METROPOLIS AWARD

Nicola Bonini (KCL), Cheol-Hwan Park (SNU), Giorgia Fugallo (Nantes), Michele Lazzeri, Lorenzo Paulatto (Paris VI), Francesco Mauri (Roma)



2D THANKS



Nicolas Mounet



Philippe Schwaller



Davide Campi



Antimo Marrazzo



Thibault Sohier



Andrius Merkys



Ivano E. Castelli



Andrea Cepellotti



Giovanni Pizzi



Nicola Marzari



ACKNOWLEDGMENTS

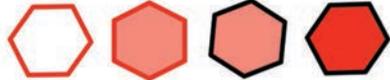


30+ in now in faculty positions and research labs worldwide:
from Harvard to MIT, Imperial College, Seoul National...



ACKNOWLEDGMENTS

MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH

<http://nccr-marvel.ch>

Swiss National Centre for Computational Design and Discovery of Novel Materials



<http://max-centre.eu>

H2020 Centre of Excellence MaX: Materials Design at the Exascale



SNSF
H2020 Nanoscience Foundries and Fine Analysis
H2020 European Materials Modelling Council

H2020 Graphene Flagship

H2020 Marketplace

H2020 EPFL Fellows

H2020 Marie Curie

Max-Planck-EPFL Centre

PASC

PRACE

Constellium

Innosuisse

Solvay

Varinor



Platform for Advanced Scientific Computing



CONCLUSIONS

- It's a very exciting and productive time for computational materials science
- Goals: Understand, predict, and design the properties and performance of novel or complex materials and devices
- Accuracy, complexity, and informatics



4 LAST WORDS OF ADVICE

1. INTELLIGENCE IS OVER-RATED – YOU NEED HARD WORK, DRIVE, VISION, CREATIVITY
2. LIFE GOES IN A BLINK
3. YOUR NEXT FEW YEARS ARE THE MOST CRITICAL
4. YOU ARE GETTING ONE OF THE BEST (ACADEMIC) EDUCATIONS IN THE WORLD