

Yonsei University Graduate Class

# **Energy Materials: Design, Discovery and Data Materials Theory and Simulation**

**Prof. Aron Walsh**

Department of Materials  
Imperial College London



<https://wmd-group.github.io>



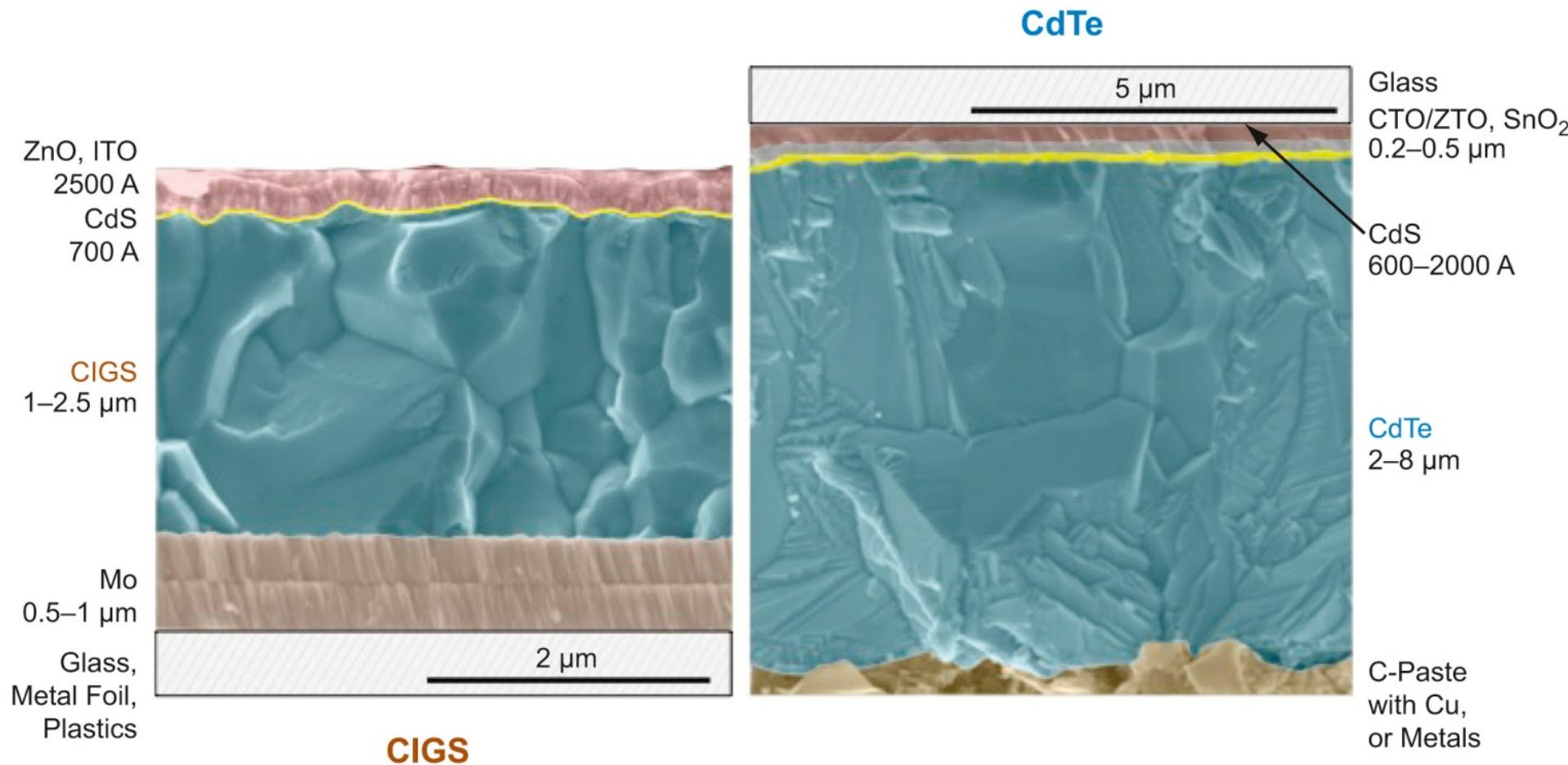
@lonepair

# Background

Materials modelling is widely used as a tool for characterisation and prediction in materials science. There is an expanding literature on energy materials (e.g. batteries, solar cells, thermoelectrics).

**Aim:** A basic understanding of terms and concepts, with the ability to critically assess research papers in your field.

# Example: Modelling Solar Cells



# Example: Modelling Solar Cells

## Front Contact

- Band offsets
- Interfacial states
- Interfacial dipoles
- Modification layers

## Device Modelling

- Carrier collection
- J-V response
- Efficiency losses
- Layer optimisation

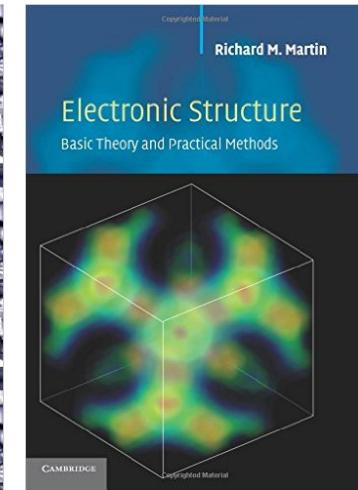
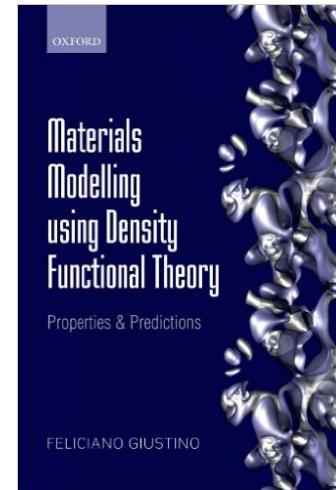
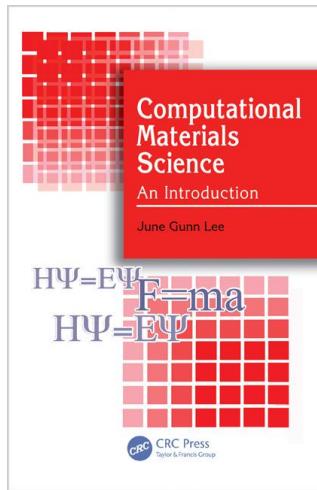
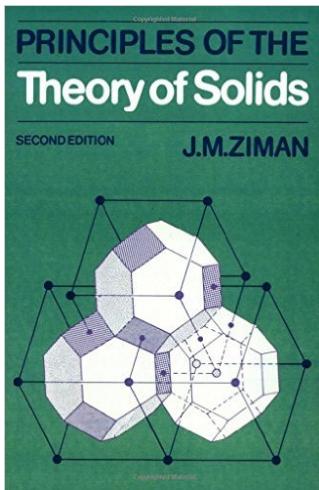
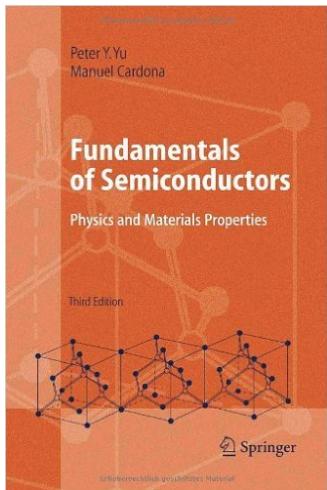
## Active Layer

- Electronic structure
- Optical properties
- Electron transport
- Defect states

## Back Contact

- Band offsets
- Ion diffusion
- Interfacial reactions
- Modification layers

# Relevant Textbooks



General

Specialist

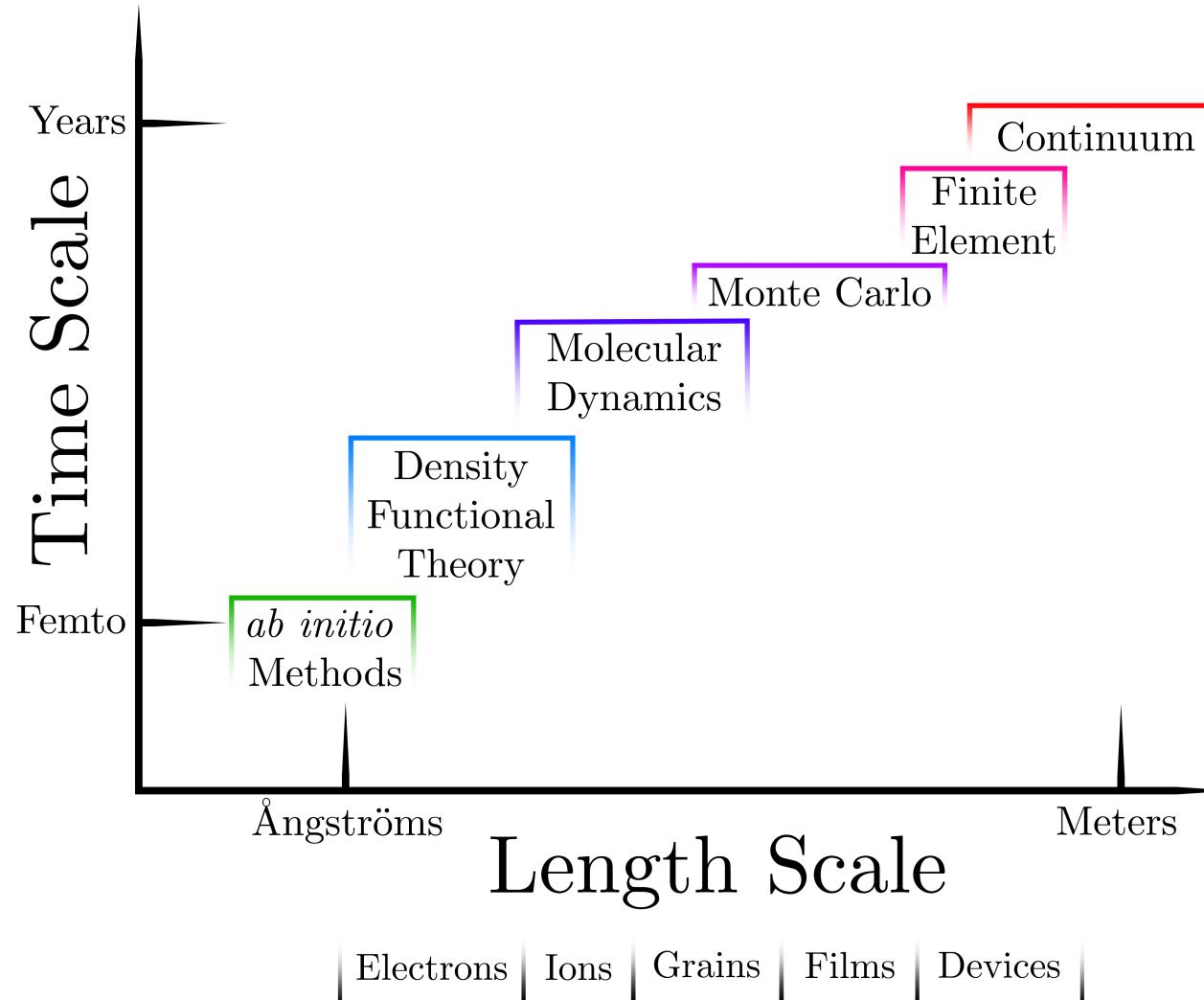


# Talk Outline: Theory and Simulation

---

- 1. Theory: What Equations to Solve**
- 2. Practice: Codes and Supercomputers**
- 3. Latest Advances: Data and Informatics**

# Multi-Scale Simulation Toolbox



# First-Principles Materials Modelling

**What?** Simulate the properties of materials using the Schrödinger equation and chemical composition as the sole input

**Why?** Accurate, unbiased and predictive

**When?** If such calculations are feasible and meaningful

**How?** Digital computers, clever algorithms, common sense and scientific rigor

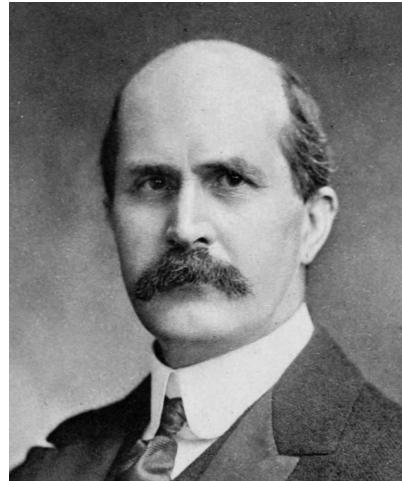
# First-Principles Workflow

Input:  
**Structure**



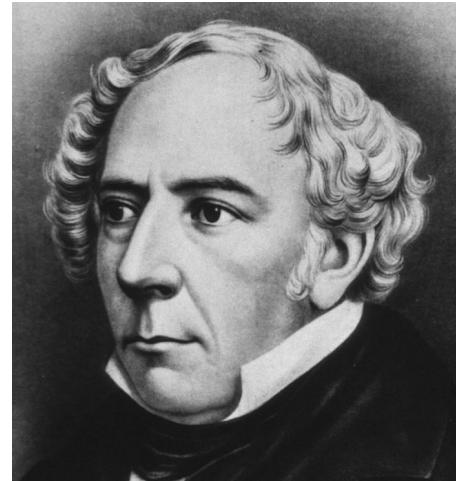
Output:  
**Properties**

X-ray Diffraction  
(unit cells)



William Bragg  
(*Wigton, 1862*)

Hamiltonian  
(ions and electrons)



William Hamilton  
(*Dublin, 1805*)

Physical Chemistry  
(stimuli)



Neville Mott  
(*Leeds, 1905*)

# Quantum Mechanics

$$\hat{H}\Psi = E\Psi$$



Kinetic and Potential Energy Operators

$$\hat{H} = \hat{T} + \hat{V}$$

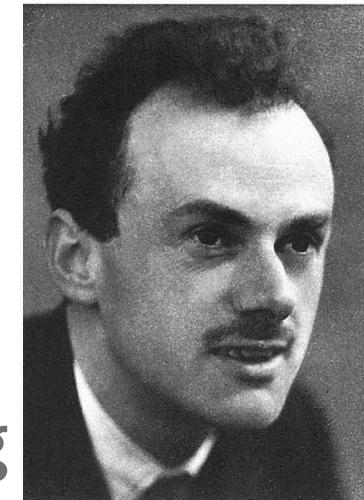
Non Relativistic

Relativistic



Schrödinger  
(1887, Vienna)

Dirac  
(1902, Bristol)  
*Extra terms:*  
scalar relativistic  
spin orbit coupling



# Electronic Structure Techniques

Wavefunction  
based quantum  
mechanics

Density based  
quantum  
mechanics

$$E[\Psi] \rightarrow E[\rho]$$

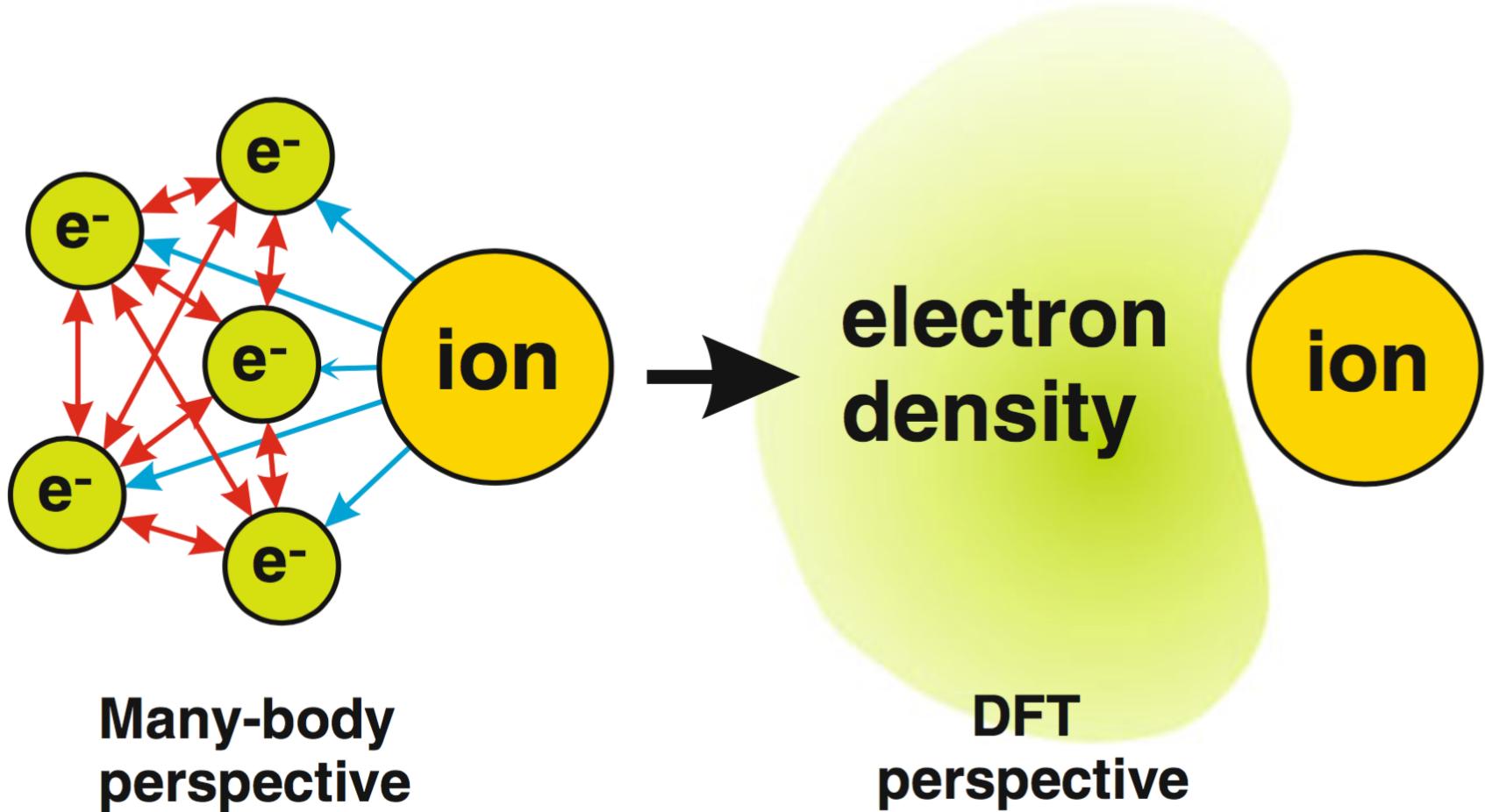
Methods

Hartree-Fock  
Møller–Plesset  
Coupled Cluster  
Configuration Interaction

Methods

Thomas–Fermi  
Density Functional  
Dynamical Mean Field  
Optimised Effective Potential

# Density Functional Theory (DFT)



# Kohn-Sham DFT (1965)

Use one-electron  $\Psi_i$  that reproduce interacting  $\rho$

**Hamiltonian**  
non-relativistic  
scalar-relativistic  
spin-orbit coupling

$$\left[ -\frac{1}{2} \nabla^2 + v_{\text{nuc}} + v_J + v_{\text{xc}} \right] \psi_i = \epsilon_i \psi_i$$

**Core Electrons**  
all-electron  
pseudopotential  
frozen-core

**Periodicity**  
0D (molecules)  
1D (wires)  
2D (surfaces)  
3D (crystals)

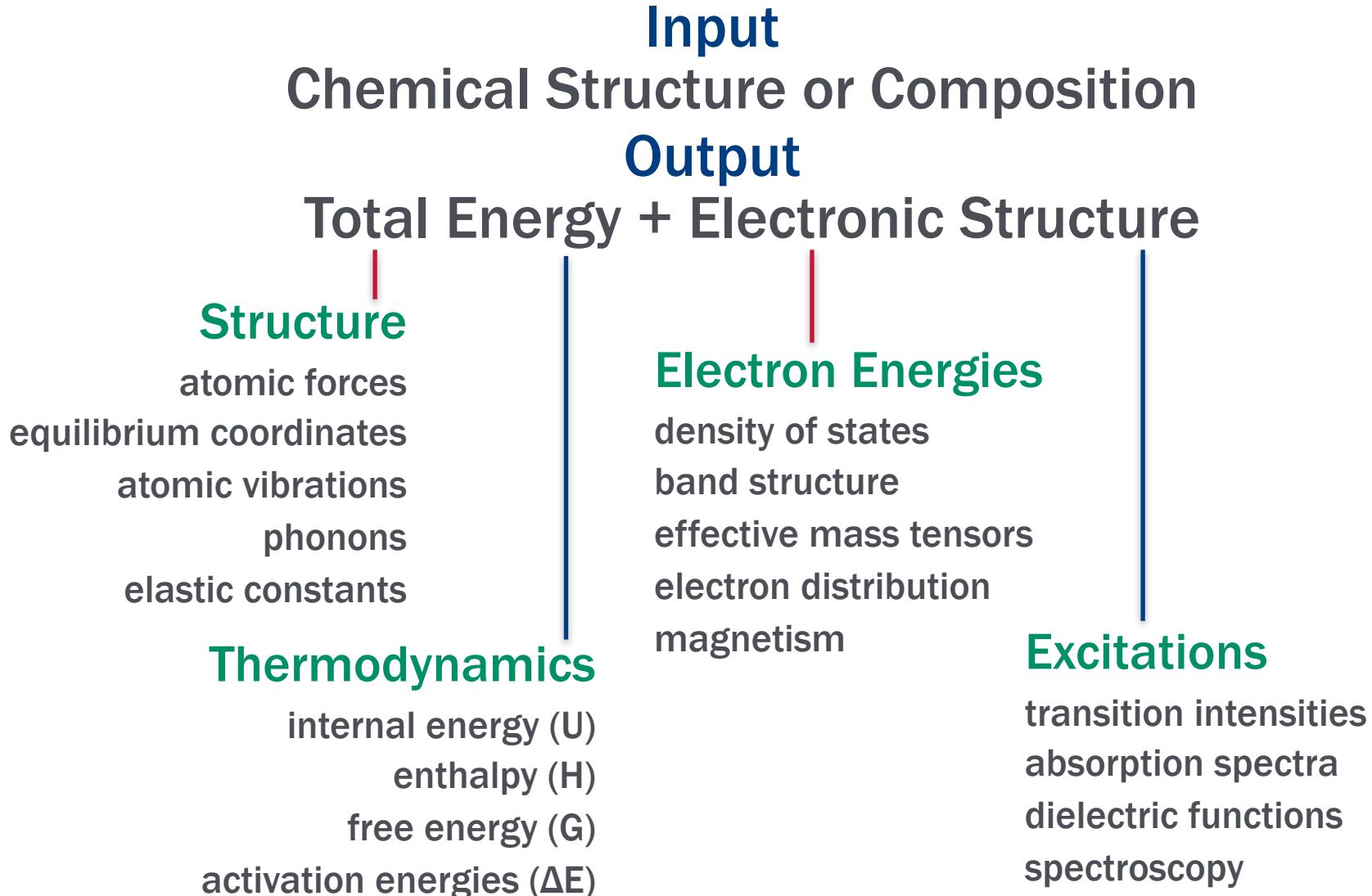
**Functional**  
beyond.....  
hybrid-GGA  
meta-GGA  
GGA  
LDA

**Electron Spin**  
restricted  
unrestricted  
non-collinear

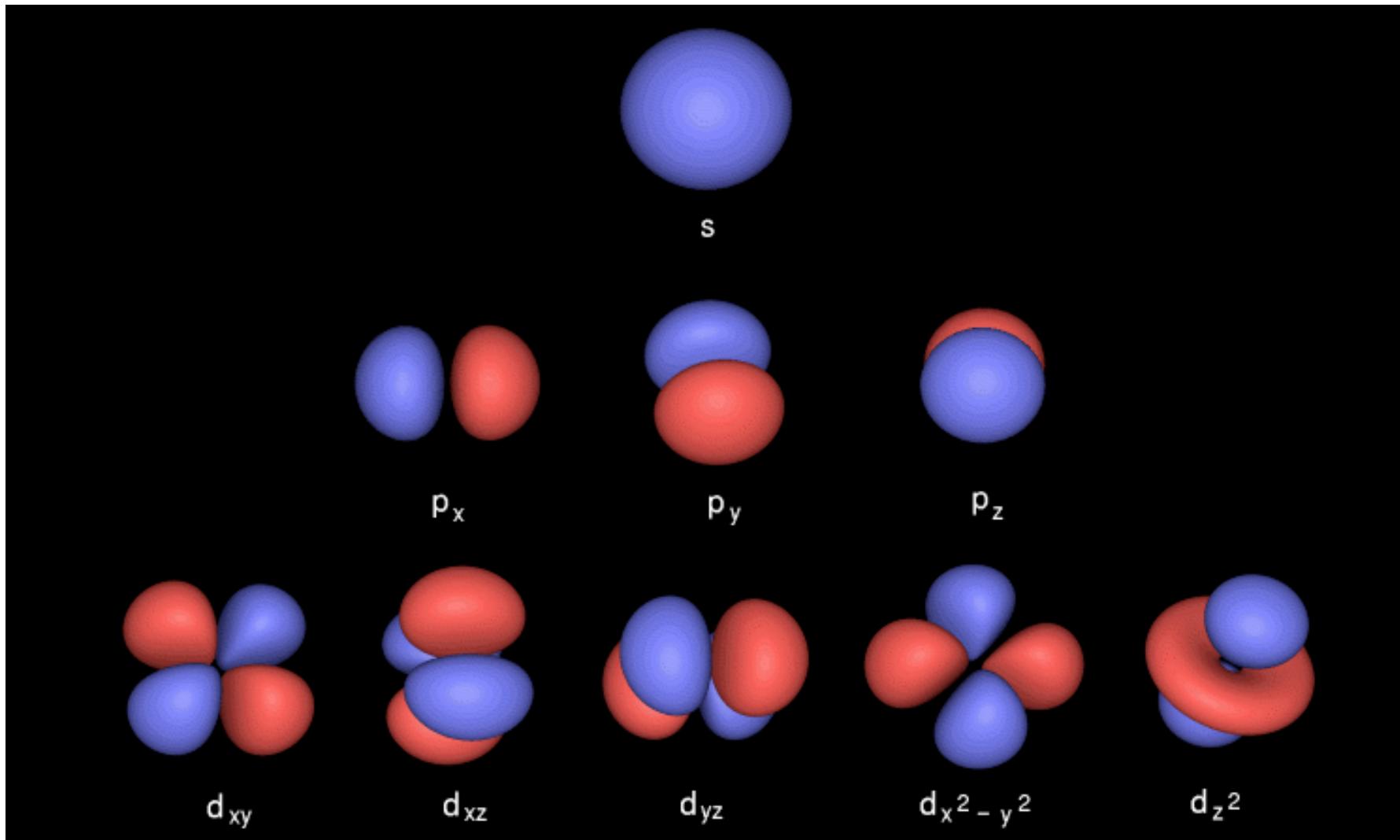
QMC  
GW  
RPA  
TD-DFT

**Basis Set**  
plane waves  
numerical orbitals  
analytical functions

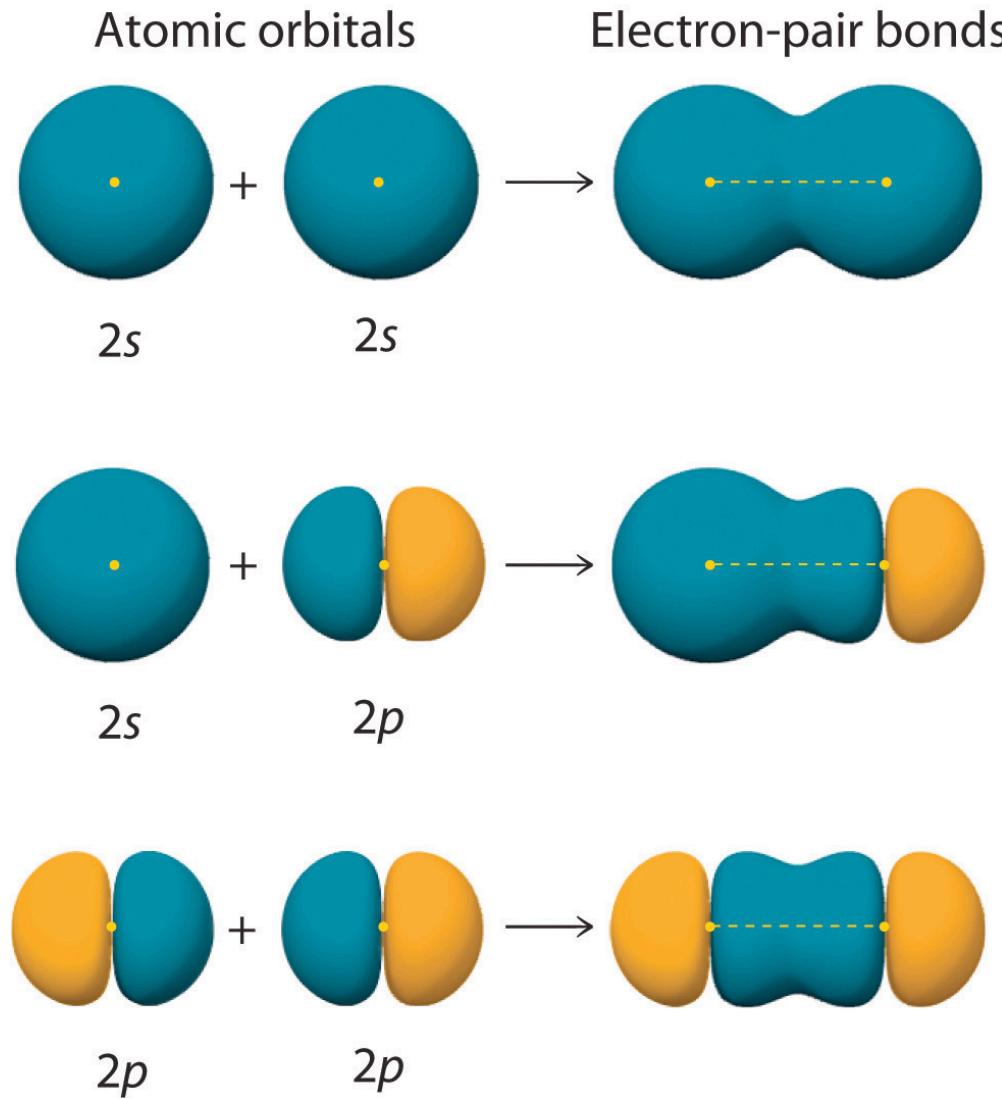
# Materials Modelling with DFT



# Exact (Analytical) Wavefunctions

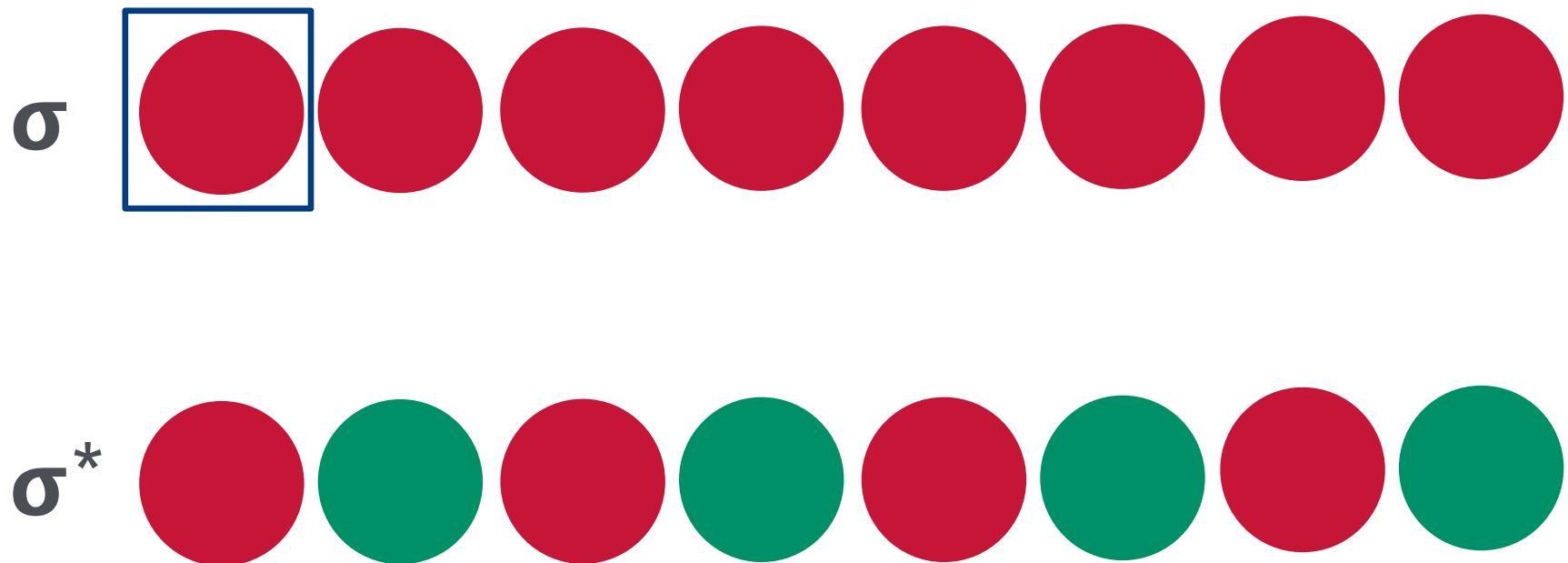


# From Atoms to Molecules

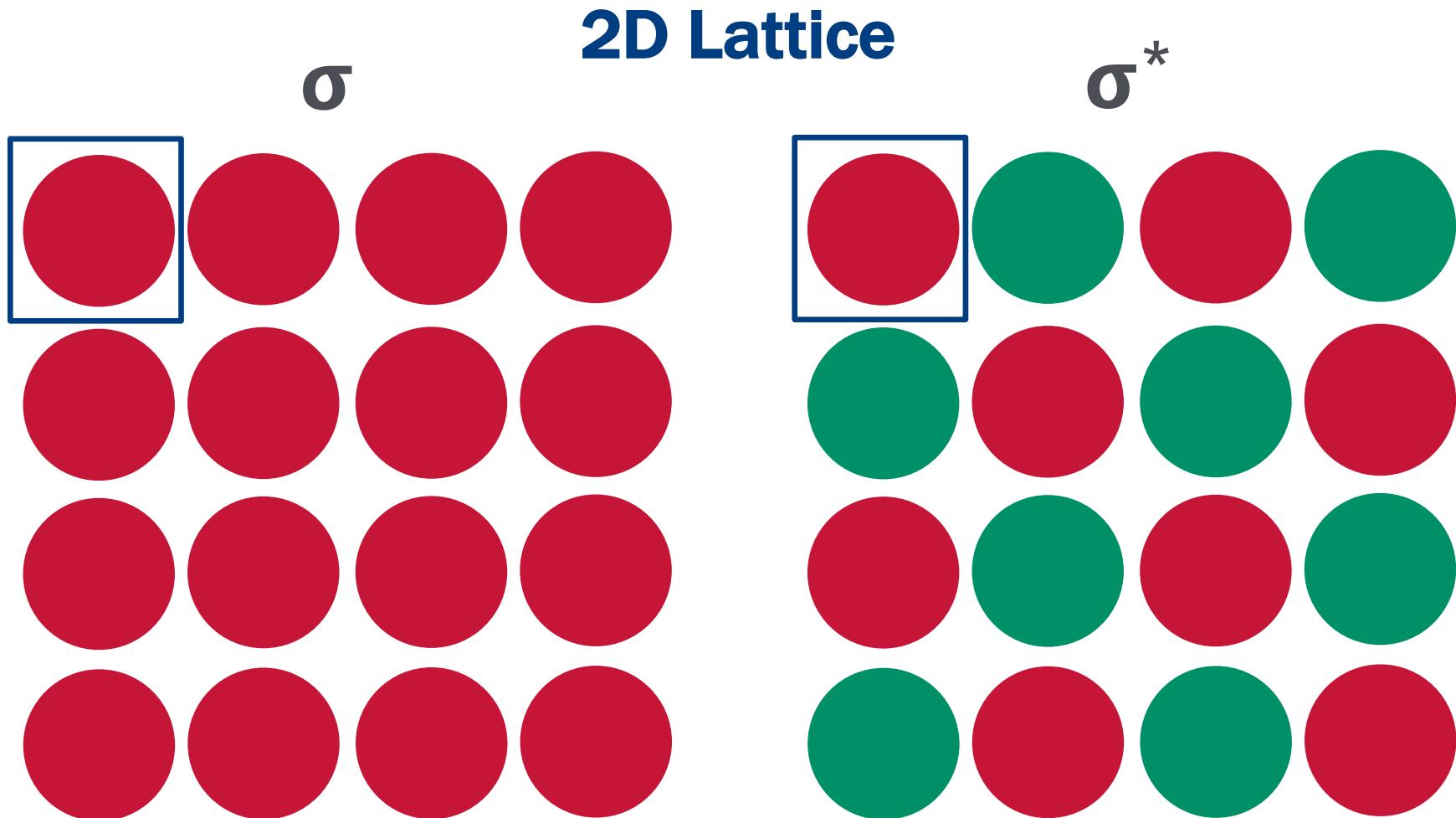


# From Molecules to 1D Chain

## 1D Chain of Atoms



# From 1D Chain to 2D Lattice



# Learn from a Laureate



Review

## How Chemistry and Physics Meet in the Solid State

Prof. Roald Hoffmann [✉](#)

First published: September 1987 [Full publication history](#)

DOI: 10.1002/anie.198708461 [View/save citation](#)

Cited by: 260 articles [Citation tools](#)



[View issue TOC](#)  
Volume 26, Issue 9  
September 1987  
Pages 846–878

### Abstract

To make sense of the marvelous electronic properties of the solid state, chemists must learn the language of solid-state physics, of band structures. An attempt is made here to demystify that language, drawing explicit parallels to well-known concepts in theoretical chemistry. To the joint search of physicists and chemists for understanding of the bonding in extended systems, the chemist brings a great deal of intuition and some simple but powerful notions. Most important among these is the idea of a bond, and the use of frontier-orbital arguments. How to find localized bonds among all those maximally delocalized bands? Interpretative constructs, such as the density of states, the decomposition of these densities, and crystal orbital overlap populations, allow a recovery of bonds, a finding of the frontier orbitals that control structure and reactivity in extended systems as well as discrete molecules.

# 3D Periodic Boundary Conditions

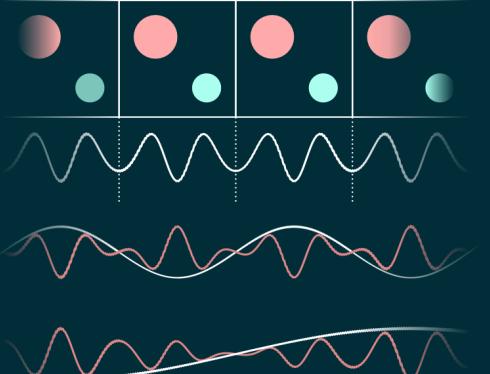
Felix Bloch (1928)

$$\Psi_k(r) = u(r)e^{ikr}$$

Crystal wavefunction

Periodic cell  
potential

Plane wave



Periodic potential

$u(r)$

$\psi(r), \mathbf{k} = (\frac{1}{2})$

$\psi(r), \mathbf{k} = (\frac{1}{8})$

Wavefunction of a particle in  
a periodic potential ( $\lambda=2\pi/k$ )

Electron wavevector  
or  
Electron momentum

# Electronic Band Structure

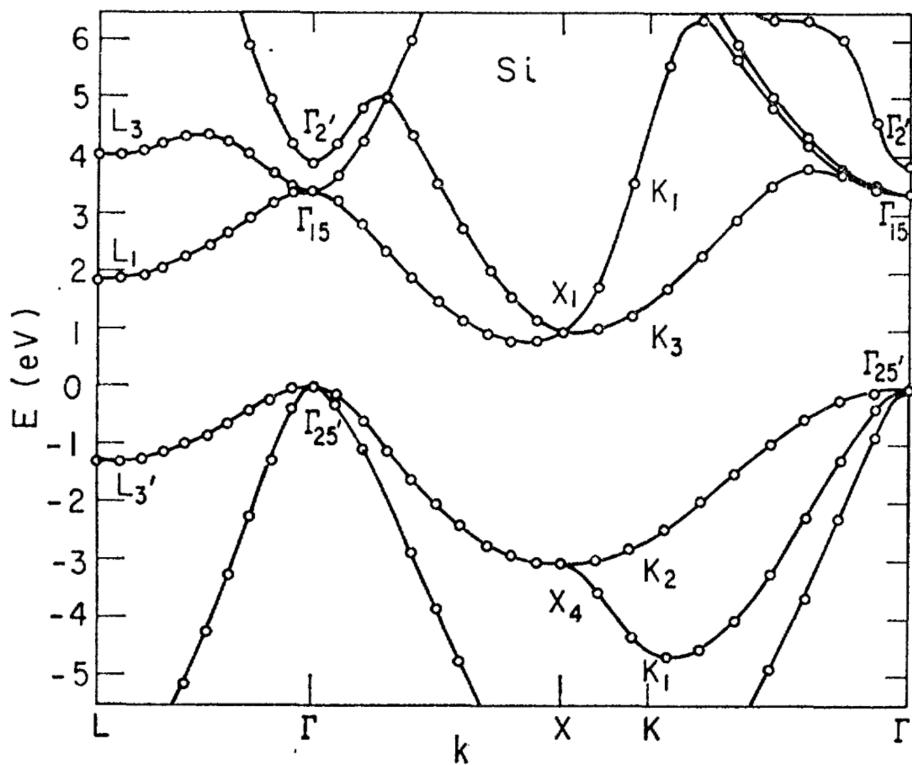
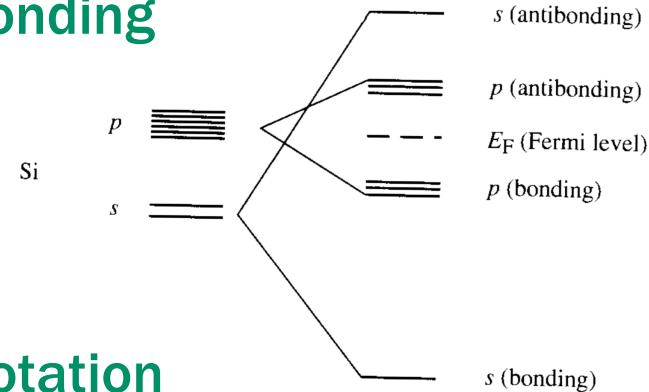


FIG. 1. Band structure of Si.

Empirical Pseudopotential Approach  
Physical Review 141, 789 (1966)

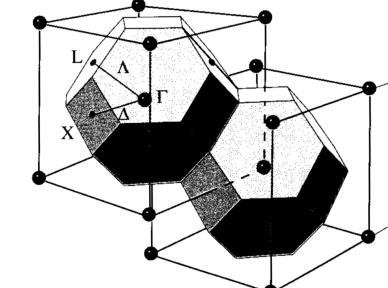
## Bonding



## Notation

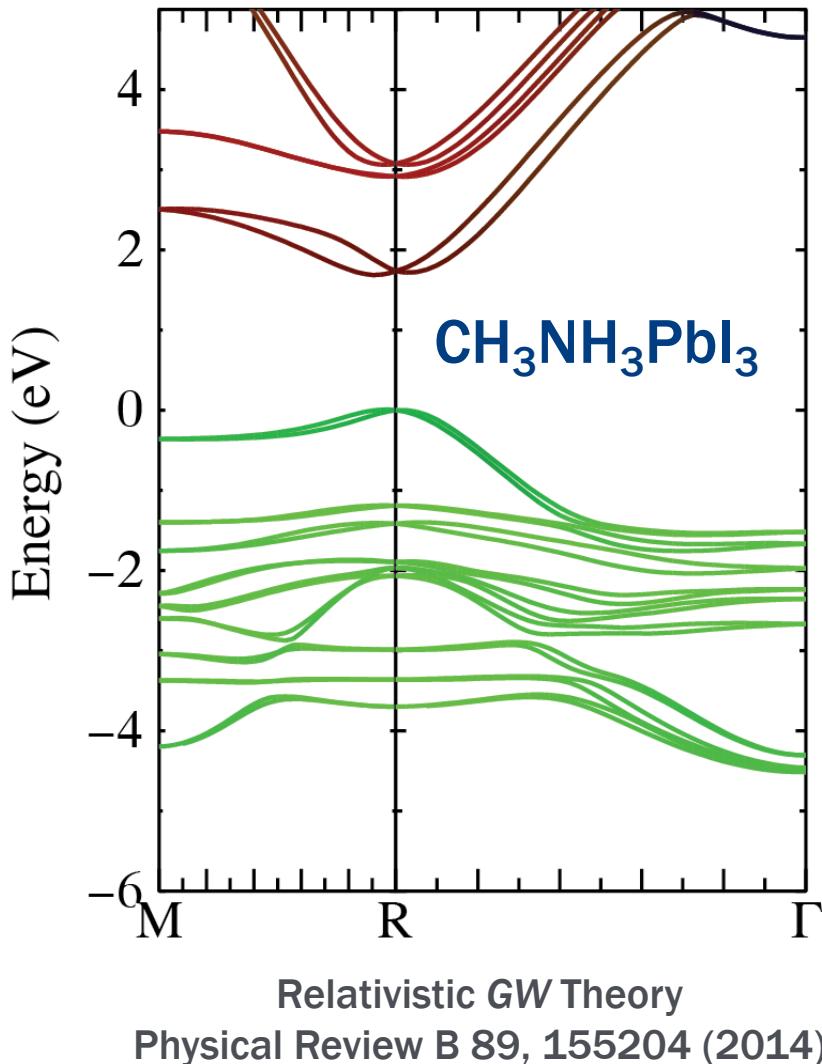
Koster notation	BSW notation	Molecular notation
$\Gamma_1$	$\Gamma_1$	$A_1$
$\Gamma_2$	$\Gamma_2$	$A_2$
$\Gamma_3$	$\Gamma_{12}$	$E$
$\Gamma_4$	$\Gamma_{15}$	$T_2$
$\Gamma_5$	$\Gamma_{25}$	$T_1$

## Brillouin Zone

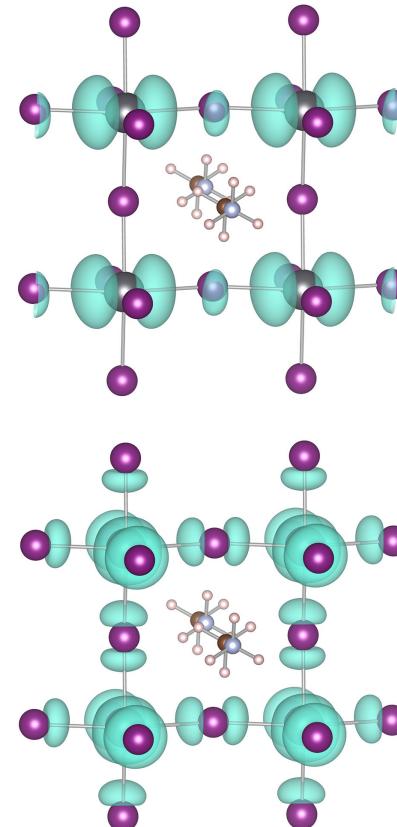


Fundamentals of Semiconductors  
Yu and Cardona (Springer, 1995)

# Electronic Band Structure



Electronic Configuration:  
 $\text{Pb}^{\text{II}} [5\text{d}^{10} \text{6s}^2 \text{6p}^0]$ ;  $\text{I}^{\text{-I}} [5\text{p}^6]$



Conduction  
Band

Valence  
Band

# Talk Outline: Theory and Simulation

---

1. Theory: What Equations to Solve
2. Practice: Codes and Supercomputers
3. Latest Advances: Data and Informatics

# Supercomputers in 2017 ( $10^{17}$ FLOPS)

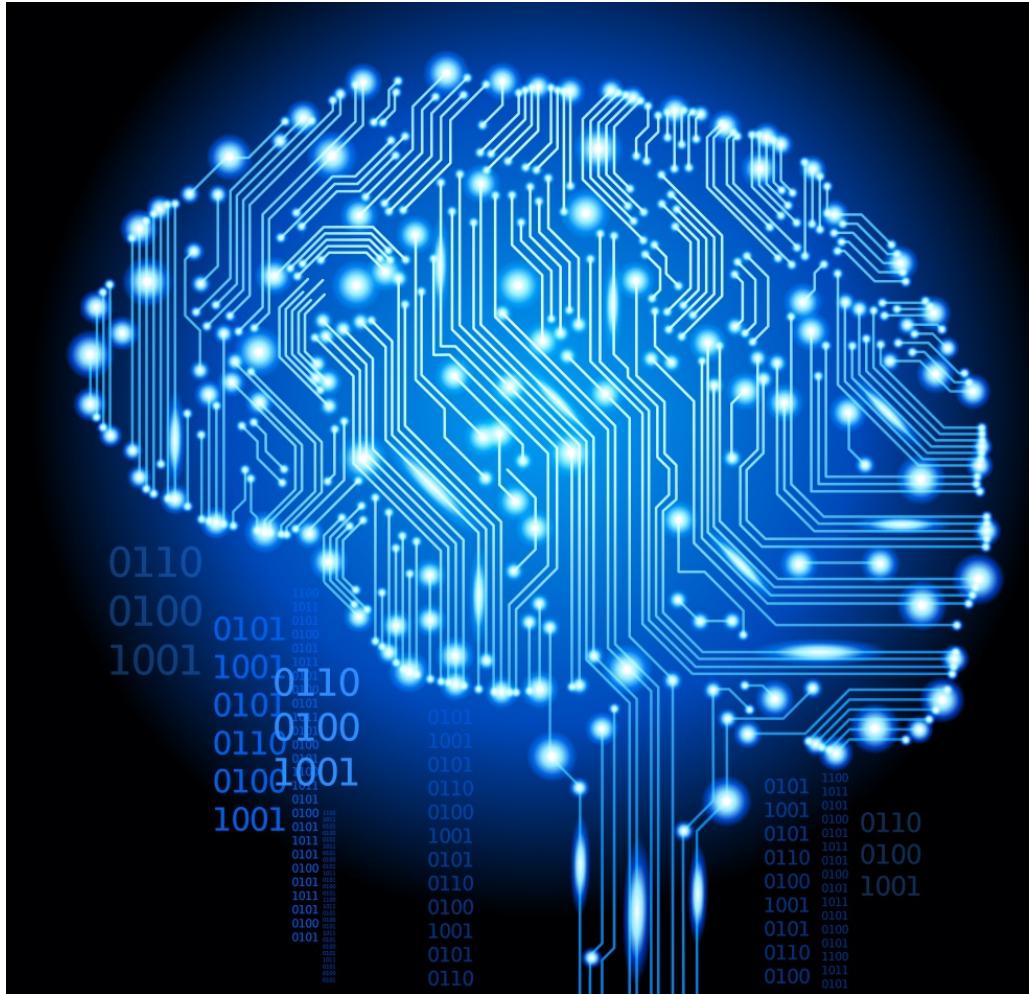
## Top500.org Ranking

### TOP 10 Sites for November 2016

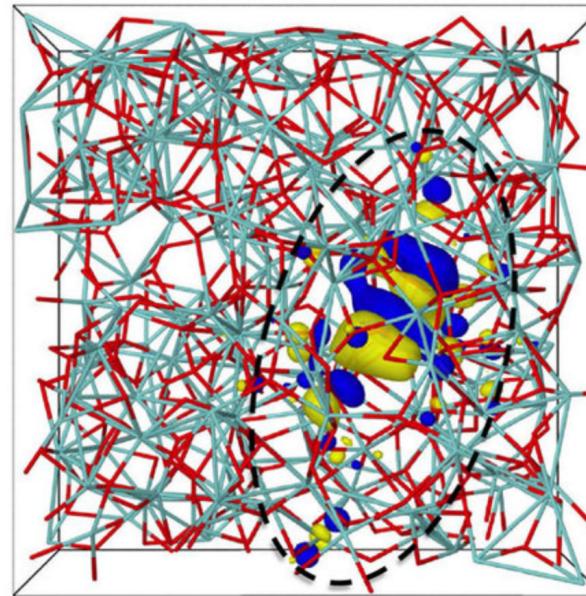
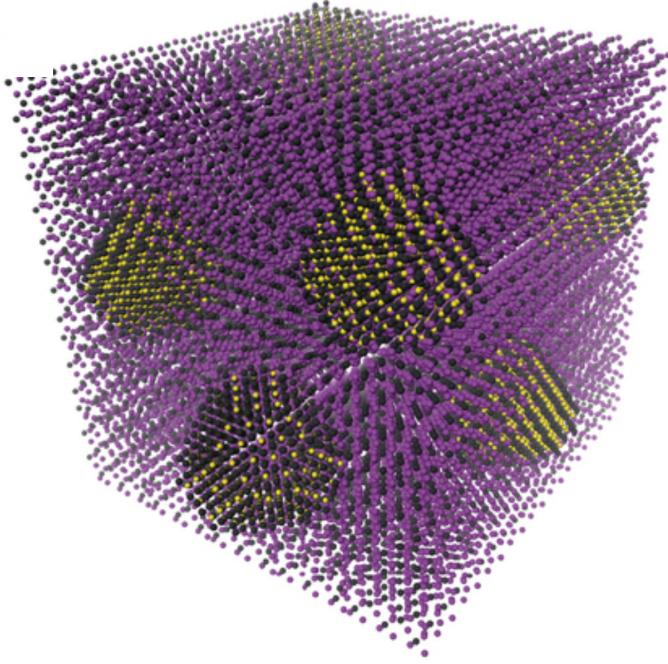
For more information about the sites and systems in the list, click on the links or view the [complete list](#).

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	<b>Sunway TaihuLight</b> - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	<b>Tianhe-2 (MilkyWay-2)</b> - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	<b>Titan</b> - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	<b>Sequoia</b> - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	DOE/SC/LBNL/NERSC United States	<b>Cori</b> - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect Cray Inc.	622,336	14,014.7	27,880.7	3,939

# Exascale Computing ( $10^{18}$ FLOPS)



# Thousands of Interacting Electrons



**“With DFT as your hammer, everything starts to look like a nail”**

Chris Pickard, 2009

# Probe Materials Chemistry and Physics

**Understanding known compounds  
and designing new materials**

**Materials Characterisation**

Bulk physical and chemical properties

**Chemical Reactions**

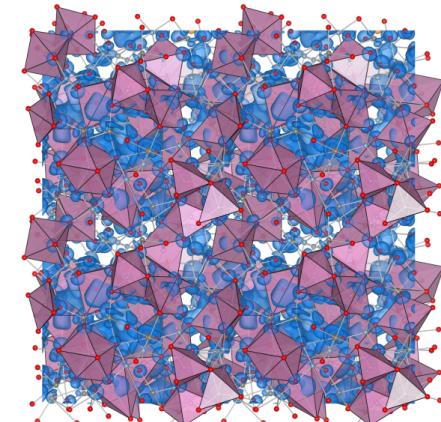
Catalysis; lattice defects; redox chemistry

**Materials Engineering**

Beneficial dopants, alloys, or morphology

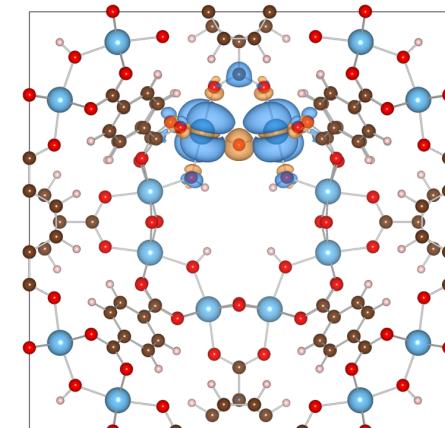
**Substrate & Device Effects**

Interfacial & strain phenomena



**Amorphisation**

Conduction states in  $\text{InGaZnO}_4$



**Hybrid Network**

Photochromic MIL-125

# First-Principles Modelling in 2017

---

**Remove Approximations**

length and times scales

electron-electron interactions

electron-phonon interactions

phonon-phonon interactions

# First-Principles Modelling in 2017

**Remove Approximations**

length and times scales

electron-electron interactions

electron-phonon interactions

phonon-phonon interactions

**Accurate Solid-State Properties**

effective mass to carrier mobility

phonon frequencies to lifetimes

ground to excited states

perfect crystals to defects and disorder

# Same Method – Same Result

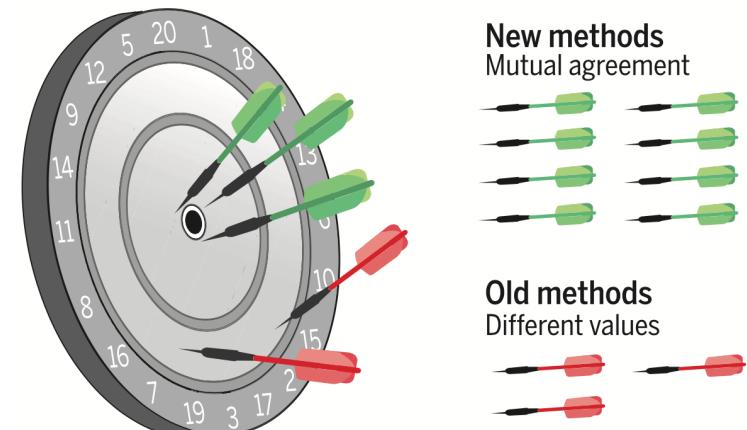
## RESEARCH ARTICLE

### DFT METHODS

## Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,<sup>1,\*</sup> Gustav Bihlmayer,<sup>2</sup> Torbjörn Björkman,<sup>3,4</sup> Peter Blaha,<sup>5</sup> Stefan Blügel,<sup>2</sup> Volker Blum,<sup>6</sup> Damien Caliste,<sup>7,8</sup> Ivano E. Castelli,<sup>9</sup> Stewart J. Clark,<sup>10</sup> Andrea Dal Corso,<sup>11</sup> Stefano de Gironcoli,<sup>11</sup> Thierry Deutsch,<sup>7,8</sup> John Kay Dewhurst,<sup>12</sup> Igor Di Marco,<sup>13</sup> Claudia Draxl,<sup>14,15</sup> Marcin Dulak,<sup>16</sup> Olle Eriksson,<sup>13</sup> José A. Flores-Livas,<sup>12</sup> Kevin F. Garrity,<sup>17</sup> Luigi Genovese,<sup>7,8</sup> Paolo Giannozzi,<sup>18</sup> Matteo Giantomassi,<sup>19</sup> Stefan Goedecker,<sup>20</sup> Xavier Gonze,<sup>19</sup> Oscar Gränäs,<sup>13,21</sup> E. K. U. Gross,<sup>12</sup> Andris Gulans,<sup>14,15</sup> François Gygi,<sup>22</sup> D. R. Hamann,<sup>23,24</sup> Phil J. Hasnip,<sup>25</sup> N. A. W. Holzwarth,<sup>26</sup> Diana Iuṣan,<sup>13</sup> Dominik B. Jochym,<sup>27</sup> François Jollet,<sup>28</sup> Daniel Jones,<sup>29</sup> Georg Kresse,<sup>30</sup> Klaus Koepernik,<sup>31,32</sup> Emine Küçükbenli,<sup>9,11</sup> Yaroslav O. Kvashnin,<sup>13</sup> Inka L. M. Locht,<sup>13,33</sup> Sven Lubeck,<sup>14</sup> Martijn Marsman,<sup>30</sup> Nicola Marzari,<sup>9</sup> Ulrike Nitzsche,<sup>31</sup> Lars Nordström,<sup>13</sup> Taisuke Ozaki,<sup>34</sup> Lorenzo Paulatto,<sup>35</sup> Chris J. Pickard,<sup>36</sup> Ward Poelmans,<sup>1,37</sup> Matt I. J. Probert,<sup>25</sup> Keith Refson,<sup>38,39</sup> Manuel Richter,<sup>31,32</sup> Gian-Marco Rignanese,<sup>19</sup> Santanu Saha,<sup>20</sup> Matthias Scheffler,<sup>15,40</sup> Martin Schlipf,<sup>22</sup> Karlheinz Schwarz,<sup>5</sup> Sangeeta Sharma,<sup>12</sup> Francesca Tavazza,<sup>17</sup> Patrik Thunström,<sup>41</sup> Alexandre Tkatchenko,<sup>15,42</sup> Marc Torrent,<sup>28</sup> David Vanderbilt,<sup>23</sup> Michiel J. van Setten,<sup>19</sup> Veronique Van Speybroeck,<sup>1</sup> John M. Wills,<sup>43</sup> Jonathan R. Yates,<sup>29</sup> Guo-Xu Zhang,<sup>44</sup> Stefaan Cottenier<sup>1,45\*</sup>

The widespread popularity of density functional theory has given rise to an extensive range of dedicated codes for predicting molecular and crystalline properties. However, each code implements the formalism in a different way, raising questions about the reproducibility of such predictions. We report the results of a community-wide effort that compared 15 solid-state codes, using 40 different potentials or basis set types, to assess the quality of the Perdew-Burke-Ernzerhof equations of state for 71 elemental crystals. We conclude that predictions from recent codes and pseudopotentials agree very well, with pairwise differences that are comparable to those between different high-precision experiments. Older methods, however, have less precise agreement. Our benchmark provides a framework for users and developers to document the precision of new applications and methodological improvements.



# A Few Popular DFT Packages

- CASTEP (Plane wave – pseudopotential)
- CP2K (Mixed Gaussian/plane wave)
- FHI-AIMS (Numeric orbitals – all electron)
- GPAW (Numeric orbitals – pseudopotential)
- QUANTUM-ESPRESSO (Plane wave – pseudopotential)
- SIESTA (Numeric orbitals - pseudopotential)
- VASP (Plane wave – pseudopotential)
- WIEN2K (Augmented plane wave – all electron)

# GPAW: Open Source and Python



<https://wiki.fysik.dtu.dk/gpaw/>

Large community of researchers. Free and open source!

- Links to Atomistic Simulation Environment
- Written in C and Python
- Easy to use
- Can be challenging to install (now: pip install gpaw)

Plane-waves	Finite-difference	LCAO
XC-functionals	DFT+U	GLLB-SC
DOS	STM	Wannier functions
delta-SCF	XAS	Jellium
TDDFT	LRTDDFT (molecules)	LRTDDFT (extended systems)
Transport	NEGF-transport	Keldysh GF-transport ...
RPA-correlation	GW	BSE
Parallelization	Continuum Solvent Model	

Lines of code:



Execution time:



# Vienna Ab Initio Simulation Package

Widely used FORTRAN code from Austria (Prof. Georg Kresse)

- License fee ~€5000 (small academic group)
- Site: <http://www.vasp.at>
- Forum: <http://cms.mpi.univie.ac.at/vasp-forum>
- Wiki: <http://cms.mpi.univie.ac.at/wiki>
- Many pre- and post-processing tools
- Visualisation: <http://jp-minerals.org/vesta>



A popular package because of reliable pseudopotentials for periodic table (benchmarked against all-electron methods)

# Compiling Scientific Codes

## General Requirements:

Program source code (e.g. **x.f**, **x.f90**, **x.c**); Makefile or configure script; Math libraries; Fortran or C compiler

## Common Compilers:

Intel Fortran (**ifort**); Portland Group (**pgf90**); Gnu-Fortran (**gfortran**); Pathscale (**pathf90**); Generic links (**f77** or **f90**)

## Common Libraries:

LAPACK (Linear algebra - diagonalisation)

- ScaLAPACK (Distributed memory version)

BLAS (Linear algebra – vector / matrix multiplication)

BLACS (Linear algebra communication subprograms)

Examples: MKL (Intel); ACML (AMD); GotoBLAS

# VASP Input Files

- **POSCAR** (“Position Card”)
- **POTCAR** (“Potential Card”)
- **INCAR** (“Input Card”)
- **KPOINTS** (k-point Sampling)

All four files should be in the same directory for VASP to run successfully

*Caution:* The order of the elements in POTCAR must be the same as POSCAR

# VASP Output Files

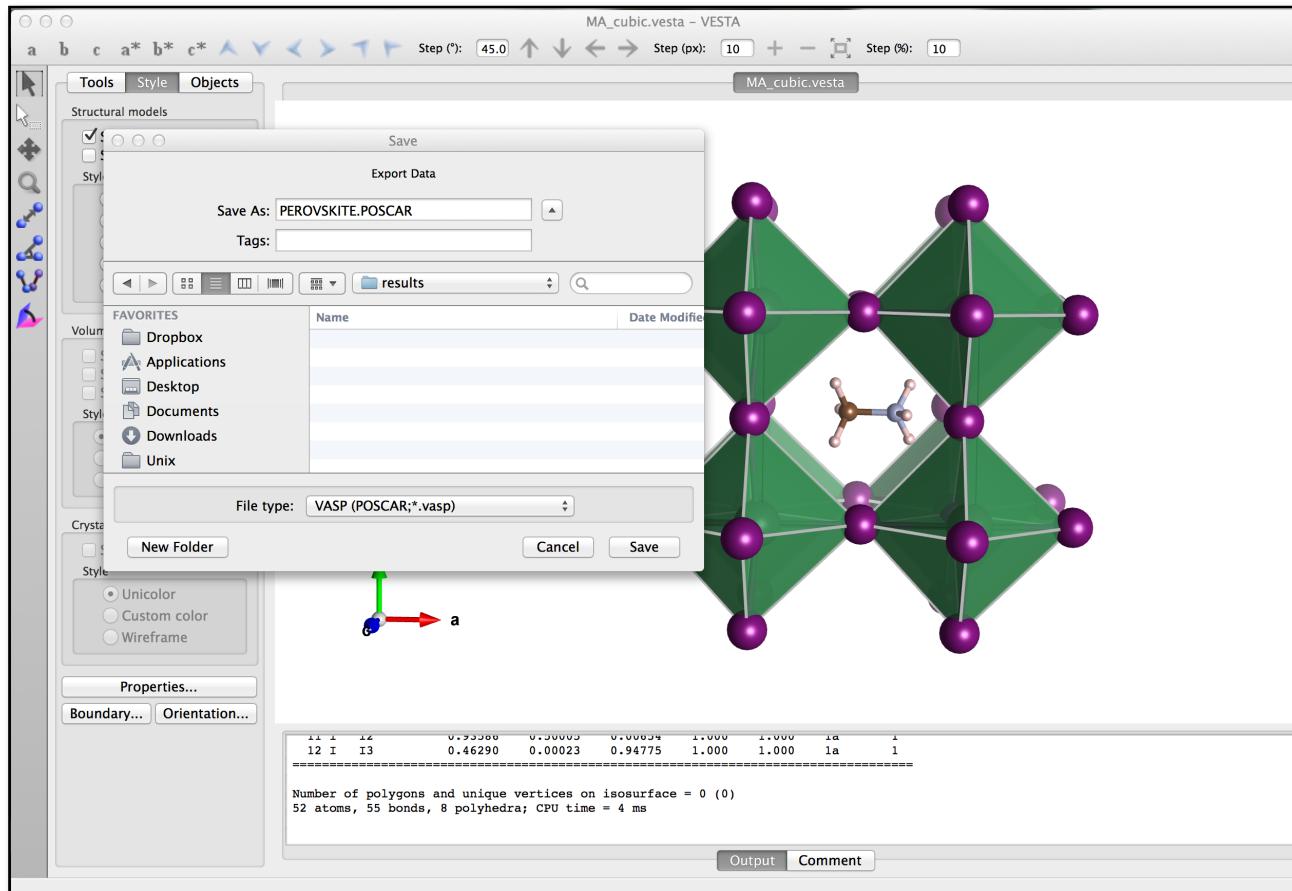
- **OUTCAR** (“Output Card”)
- **CONTCAR** (“Continue [Positions] Card”)
- **CHGCAR** (“Charge Density Card”)
- **vasprun.xml** (Auxiliary output as xml)

A number of additional files that are generated depending on flags set in INCAR

*Caution:* If NSW > 0, a number of the properties are averaged over past structures (rerun with NSW=0 at end)

# Step 1: Structure

Generate crystal structure by hand, from supplementary information, or from a database (e.g. ICSD)



# Step 1: Structure

## Check POSCAR

```
PEROVSKITE.POSCAR.vasp — results
PEROVSKITE.POSCAR.vasp

1 MA-PbI3
2 1.0
3      6.2899999619      0.0000000000      0.0000000000
4      0.0000000000      6.2899999619      0.0000000000
5      0.0000000000      0.0000000000      6.2899999619
6      C      N      H      Pb      I
7      1      1      6      1      3
8 Direct
9      0.402779996      0.499962986      0.496335000
10     0.636582971      0.499826998      0.524878025
11     0.364508003      0.499713004      0.325735003
12     0.337794006      0.643756986      0.571928024
13     0.337588996      0.356516004      0.572382987
14     0.707588017      0.634274006      0.458133996
15     0.707392991      0.365063012      0.458496988
16     0.682012975      0.500002980      0.685352981
17     0.976171017      0.000031000      0.975646973
18     0.926802993      0.999882996      0.472609013
19     0.935859978      0.500045002      0.006542000
20     0.462897986      0.000227000      0.947746992
21
```

Line: 1:9 | Plain Text ▲ | Tab Size: 4 ▼ | ⚙ ▲ | ▾ | ●

## Step 2: Input Files

```
[aron@wmd-master input]$ ls
total 1000
-rw-r--r-- 1 aron      1656 Mar 23 12:17 POSCAR
-rw-r--r-- 1 aron      1789 Mar 23 12:17 INCAR
-rw-r--r-- 1 aron 1009894 Mar 23 12:17 POTCAR
-rw-r--r-- 1 aron       49 Mar 23 12:17 KPOINTS
```

```
cat ./C/POTCAR ./N/POTCAR ./H/POTCAR ./Pb_d/POTCAR ./I/POTCAR > POTCAR
```

<b>!Ionic Relaxation:</b>	<b>INCAR (Partial)</b>
EDIFFG = -0.005	(Ionic convergence eV/A)
NSW = 0	(Max steps)
NBLOCK = 1	(Update XDATCAR/DOSCAR every X steps)
IBRION = 1	(Algorithm: 0-MD, 1-Quasi-New, 2-CG)
ISIF = 2	(Stress/Relaxation: 2-Ions, 3-Shape/Ions/V, 7-Vol)
ISYM = 2	(Symmetry: Use all)
ISMEAR = 0	(Gaussian smearing)
SIGMA = 0.001	(Smearing in eV; Metals:0.2)

Automatic mesh	<b>KPOINTS</b>
0	
Gamma	
6 6 6	
0. 0. 0.	]

# Step 3: Run VASP

---

Let's see...

# Choice of $E_{xc}$ Takes Experience

TABLE V. Lattice constant (Å) and band gap (eV) results for the SC/40 test set. (a) and (c) denote the two different lattice constants for wurzite.

Solid	Lattice constants					Band gaps				
	LSDA	PBE	TPSS	HSE	Expt.	LSDA	PBE	TPSS	HSE	Expt.
C	3.537	3.579	3.579	3.553	3.567	4.23	4.17	4.21	5.49	5.48
Si	5.410	5.479	5.466	5.444	5.430	0.59	0.75	0.82	1.28	1.17
Ge	5.634	5.776	5.744	5.701	5.658	0.00	0.00	0.00	0.56	0.74
SiC	4.355	4.404	4.394	4.372	4.358	1.40	1.46	1.42	2.39	2.42
BN	3.584	3.629	3.629	3.603	3.616	4.45	4.51	4.52	5.98	6.22
BP	4.509	4.567	4.566	4.543	4.538	1.31	1.41	1.45	2.16	2.4
BAs	4.750	4.829	4.821	4.794	4.777	1.16	1.27	1.29	1.92	1.46
BSb	5.201	5.291	5.280	5.251	n/a	0.80	0.88	0.81	1.37	n/a
AlN	(a)	3.112	3.153	3.147	3.127	3.111	4.98	4.95	5.01	6.45
	(c)	4.974	5.045	5.028	5.000	4.981				6.13
AlP	5.436	5.508	5.497	5.472	5.463	1.60	1.83	1.90	2.52	2.51
AlAs	5.639	5.733	5.713	5.691	5.661	1.40	1.62	1.71	2.24	2.23
AlSb	6.079	6.188	6.172	6.146	6.136	1.29	1.40	1.63	1.99	1.68
GaN	(a)	3.167	3.233	3.224	3.198	3.189	2.09	1.70	1.73	3.21
	(c)	5.165	5.272	5.244	5.204	5.185				3.50
$\beta$ -GaN	4.476	4.569	4.552	4.518	4.523	1.93	1.55	1.56	3.03	3.30
GaP	5.418	5.534	5.522	5.484	5.451	1.59	1.71	1.98	2.47	2.35
GaAs	5.626	5.771	5.745	5.705	5.648	0.43	0.19	0.52	1.21	1.52
GaSb	6.043	6.208	6.183	6.140	6.096	0.09	0.00	0.08	0.72	0.73
InN	(a)	3.523	3.599	3.589	3.555	3.537	0.02	0.01	0.00	0.71
	(c)	5.684	5.807	5.765	5.729	5.704				0.69

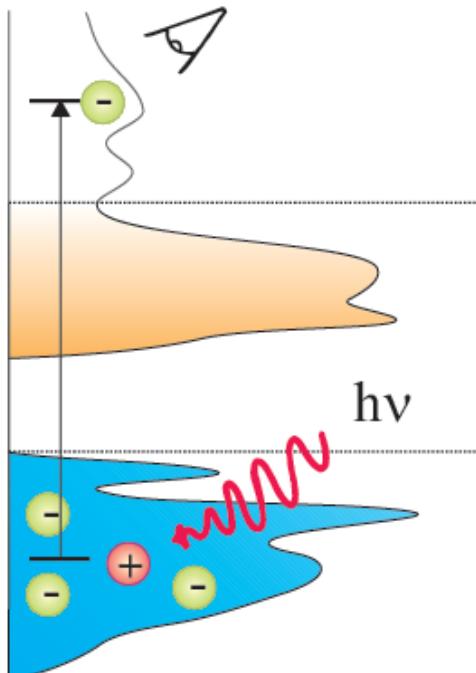
**Recommended: PBEsol (GGA for solids) & HSE06 (screened hybrid GGA)**

Journal of Chemical Physics 123, 174101 (2005)

# Electronic Spectroscopy

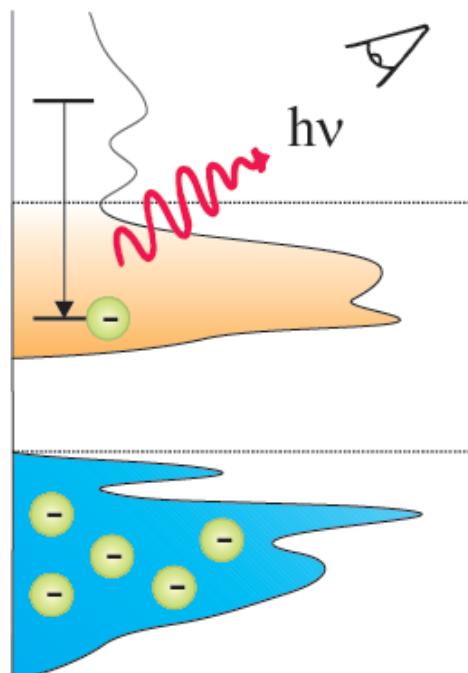
Electronic band gap  $\neq$  Optical band gap

Photoemission



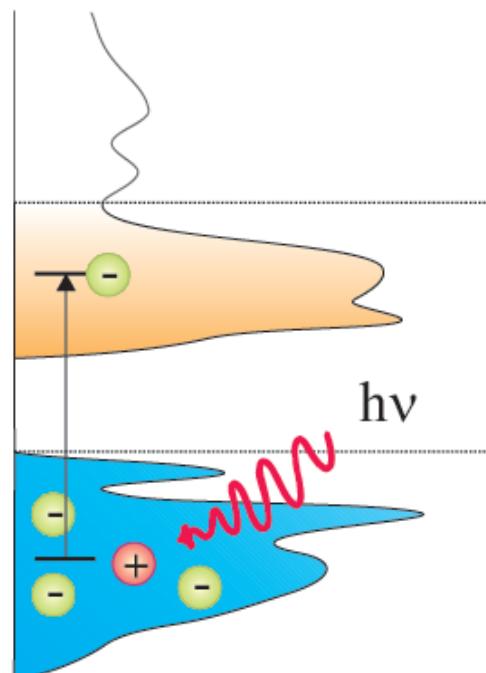
N-1 quasi-particle  
(electron + interaction with environment)

Inverse Photoemission



N+1 quasi-particle

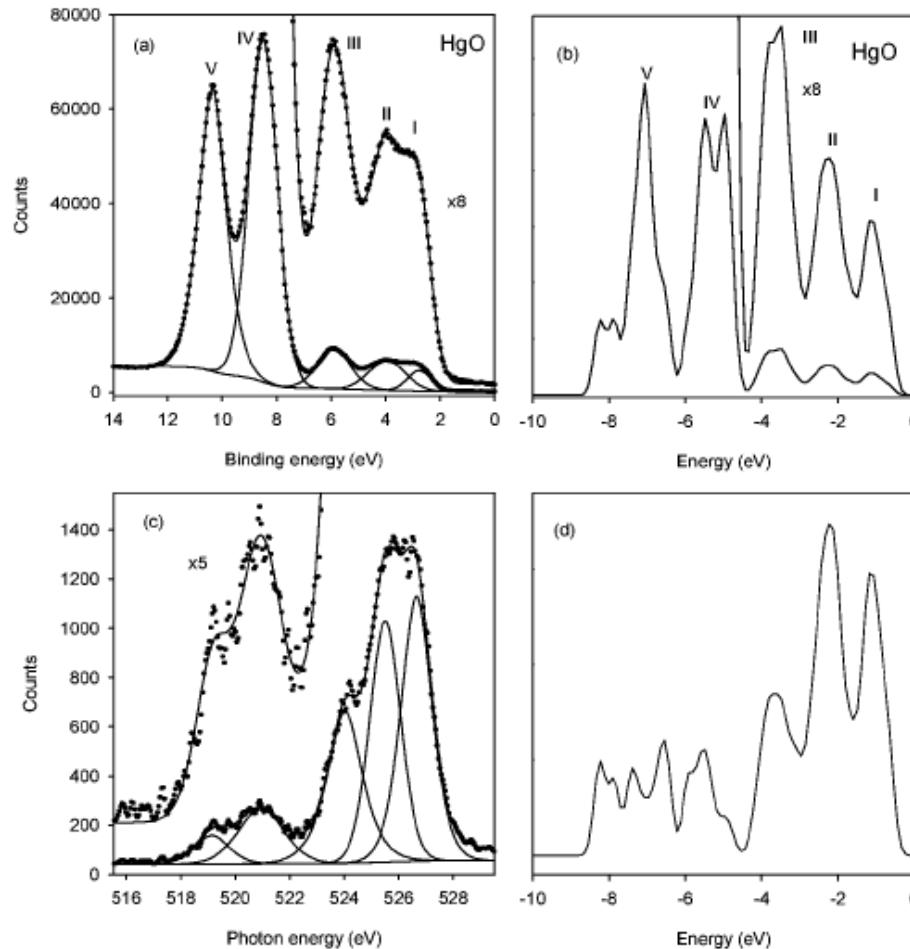
Absorption



N excitation  
(e-h interaction)

Source: Patrick Rinks (FHI-AIMS Workshop 2011)

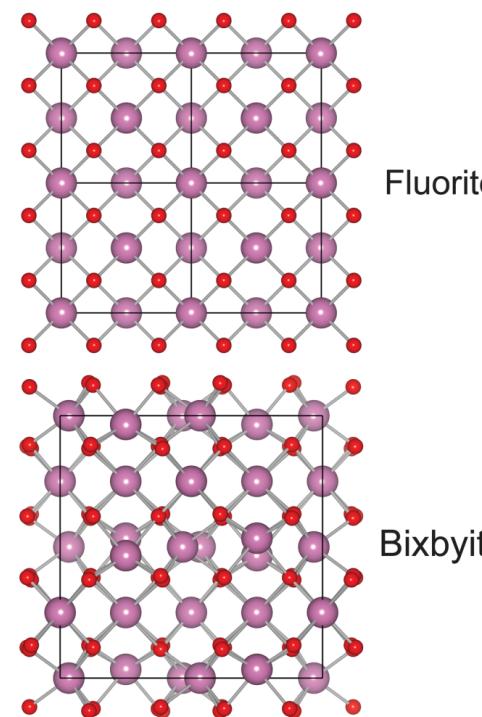
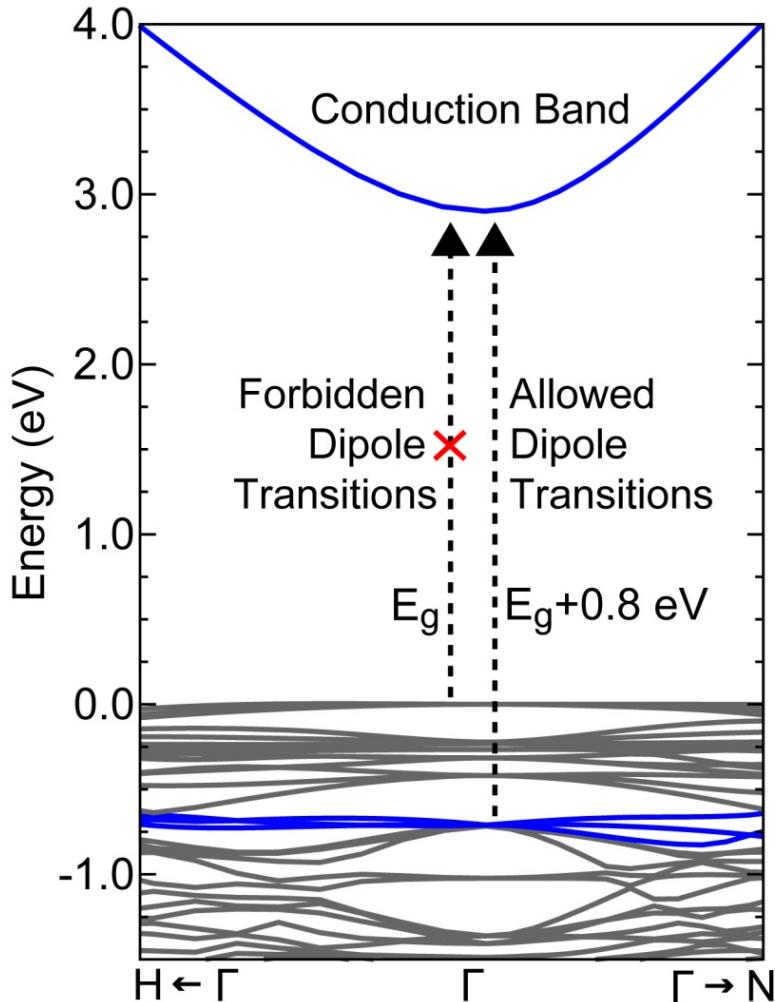
# Electronic Spectroscopy: HgO



XPS  
(weighted DOS)

O K XES  
(O 2p DOS)

# Electronic vs Optical: $\text{In}_2\text{O}_3$



# Talk Outline: Theory and Simulation

---

- 1. Theory: What Equations to Solve**
- 2. Practice: Codes and Supercomputers**
- 3. Latest Advances: Data and Informatics**

# Past: Local Optimisation

**INPUT**

Structure

**OUTPUT**

Properties

# Present: Global Optimisation

**INPUT**

Composition

**OUTPUT**

Structure

# Future: Materials Design

**INPUT**

Property

**OUTPUT**

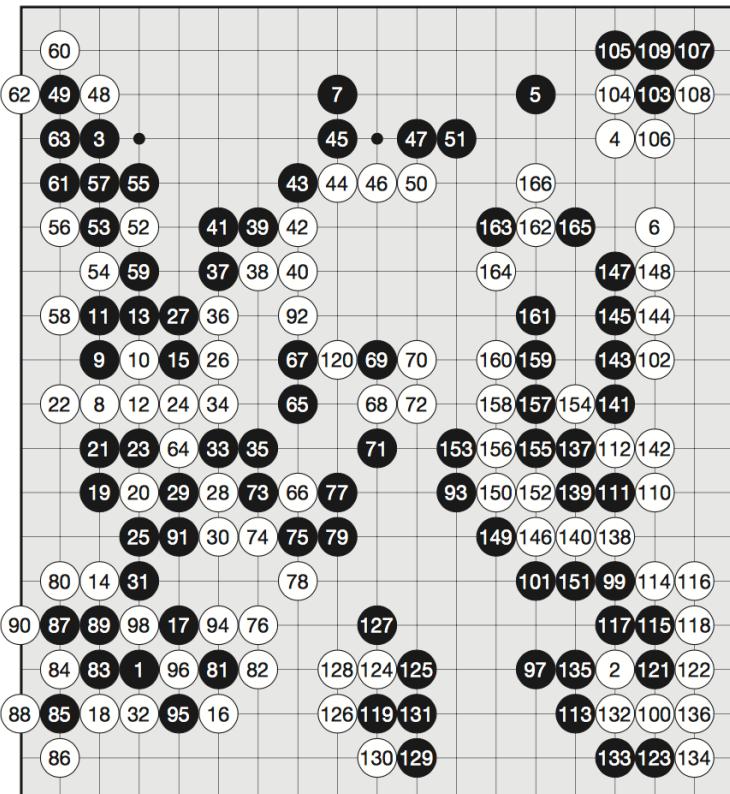
Composition  
Structure

# Games Are Fun (And Useful)



# Combinatorial Explosion

Fan Hui (Black), AlphaGo (White)  
AlphaGo wins by resignation



- **$19 \times 19$  grid**
- **Black, white, empty**
- **$3^{361} = 10^{172}$**

~  **$10^{80}$  atoms in the universe**

# Alpha Go

## ARTICLE

doi:10.1038/nature16961

# Mastering the game of Go with deep neural networks and tree search

David Silver<sup>1\*</sup>, Aja Huang<sup>1\*</sup>, Chris J. Maddison<sup>1</sup>, Arthur Guez<sup>1</sup>, Laurent Sifre<sup>1</sup>, George van den Driessche<sup>1</sup>, Julian Schrittwieser<sup>1</sup>, Ioannis Antonoglou<sup>1</sup>, Veda Panneershelvam<sup>1</sup>, Marc Lanctot<sup>1</sup>, Sander Dieleman<sup>1</sup>, Dominik Grewe<sup>1</sup>, John Nham<sup>2</sup>, Nal Kalchbrenner<sup>1</sup>, Ilya Sutskever<sup>2</sup>, Timothy Lillicrap<sup>1</sup>, Madeleine Leach<sup>1</sup>, Koray Kavukcuoglu<sup>1</sup>, Thore Graepel<sup>1</sup> & Demis Hassabis<sup>1</sup>

The game of Go has long been viewed as the most challenging of classic games for artificial intelligence owing to its enormous search space and the difficulty of evaluating board positions and moves. Here we introduce a new approach to computer Go that uses ‘value networks’ to evaluate board positions and ‘policy networks’ to select moves. These deep neural networks are trained by a novel combination of supervised learning from human expert games, and reinforcement learning from games of self-play. Without any lookahead search, the neural networks play Go at the level of state-of-the-art Monte Carlo tree search programs that simulate thousands of random games of self-play. We also introduce a new search algorithm that combines Monte Carlo simulation with value and policy networks. Using this search algorithm, our program AlphaGo achieved a 99.8% winning rate against other Go programs, and defeated the human European Go champion by 5 games to 0. This is the first time that a computer program has defeated a human professional player in the full-sized game of Go, a feat previously thought to be at least a decade away.

<https://deepmind.com>

# Alpha Go Master (Superhuman)



Demis Hassabis

@demishassabis

Follow

Excited to share an update on #AlphaGo!



04/01/17

We've been hard at work improving AlphaGo, and over the past few days we've played some unofficial online games at fast time controls with our new prototype version, to check that it's working as well as we hoped. We thank everyone who played our accounts Magister(P) and Master(P) on the Tygem and FoxGo servers, and everyone who enjoyed watching the games too! We're excited by the results and also by what we and the Go community can learn from some of the innovative and successful moves played by the new version of AlphaGo.

Having played with AlphaGo, the great grandmaster Gu Li posted that, "Together, humans and AI will soon uncover the deeper mysteries of Go". Now that our unofficial testing is complete, we're looking forward to playing some official, full-length games later this year in collaboration with Go organisations and experts, to explore the profound mysteries of the game further in this spirit of mutual enlightenment. We hope to make further announcements soon!

RETWEETS  
2,989 LIKES  
2,894



Late 2016:  
**Master beat the world number one player Ke Jie twice, and won 50 out of 51 games that it played**

# Inside Alpha-Go

**Uses machine learning to avoid the need for expert knowledge to be coded**

Space of allowed models

Scoring function

Search algorithm

**REPRESENTATION**

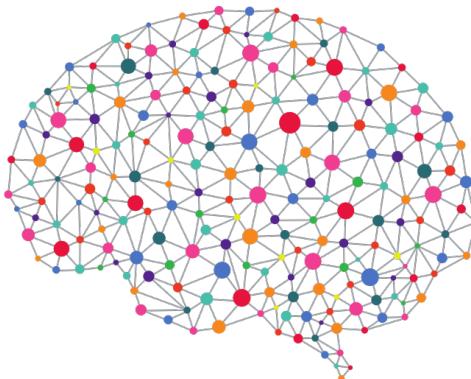
**EVALUATION**

**OPTIMIZATION**

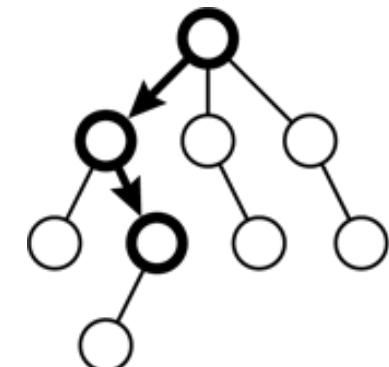
Deep neural network

Likelihood of winning

Monte Carlo tree search



<https://deepmind.com>

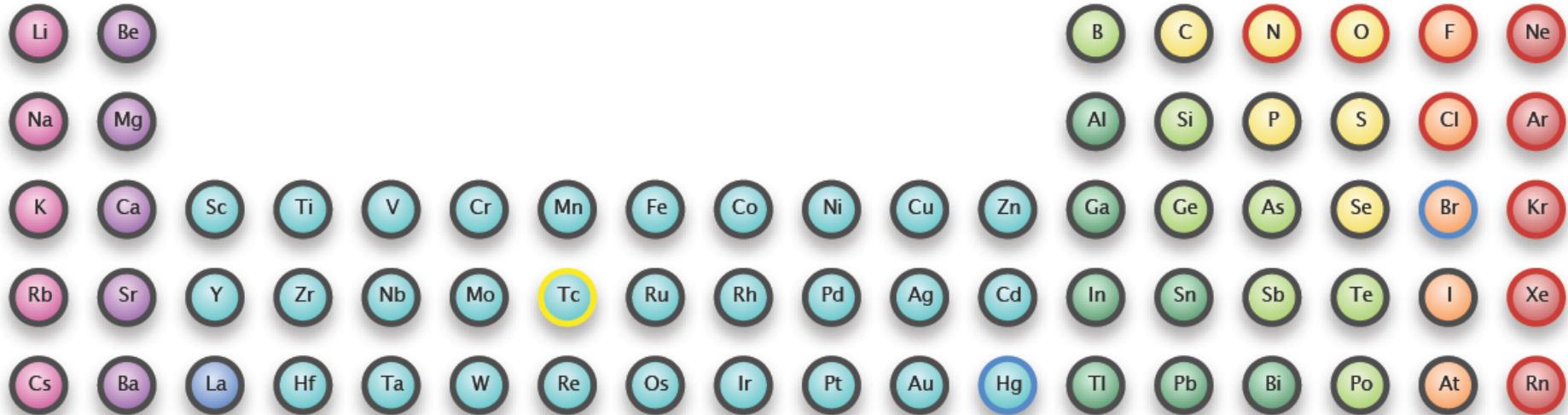


# From 2D Grid to 3D Lattice

---

- $19 \times 19$  grid
  - Black, white, empty
  - $3^{361} = 10^{172}$
- 
- $10 \times 10 \times 10$  lattice
  - 50 elements
  - $50^{1000} = 10^{1968}$

# Materials Hyperspace



Type and ratio of ions with their arrangement in space

How to find the optimal materials for:  
Property / Performance / Sustainability

# Computational Materials Design

INPUT	OUTPUT
Property	Composition Structure

- Chemical heuristics
- High-throughput screening
- Data mining
- Machine learning

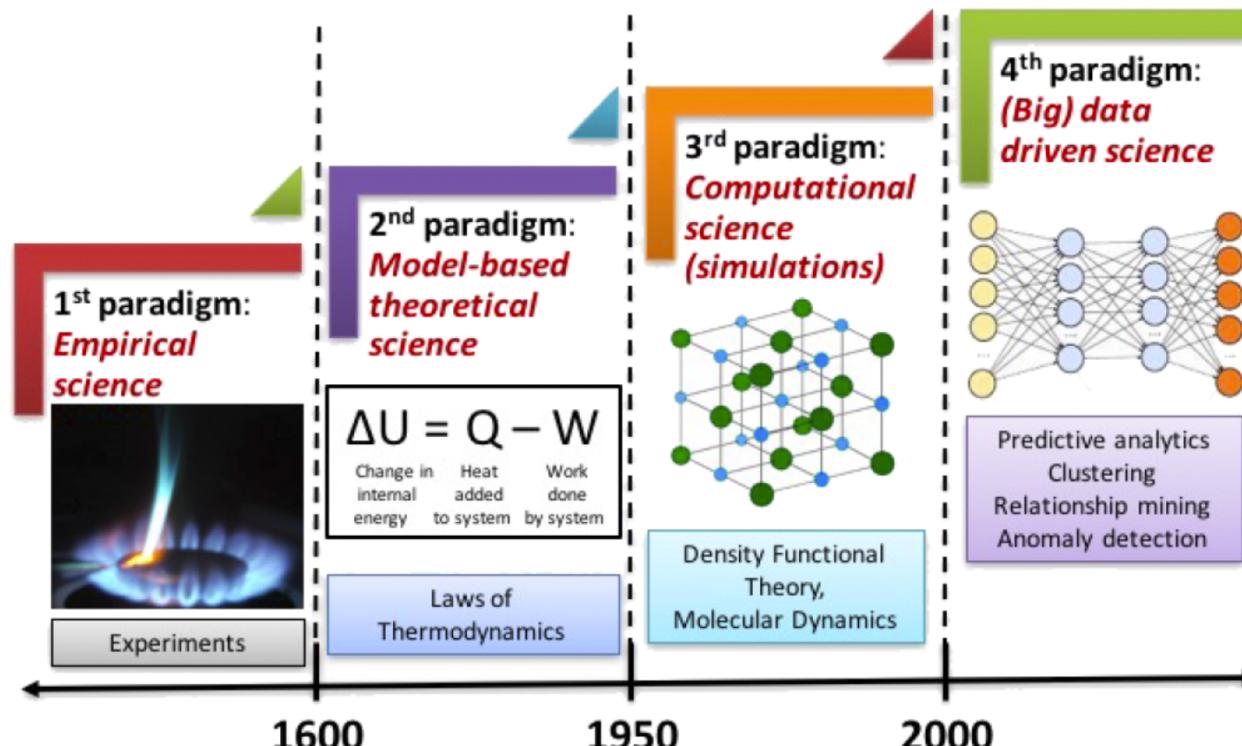
# Computational Materials Design

INPUT	OUTPUT
Property	Composition Structure

- Chemical heuristics
  - High-throughput screening
  - Data mining
  - Machine learning
- 
- “Materials  
Genome”

# New Paradigm in Science

## Global Movement Associated with Databases, #OpenData and #OpenScience



# Thermoelectrics: Heat to Electricity

Thermoelectrics Design Lab

Materials Visualization Resources Contribute

**Parameters** [?](#)

**Space Group**

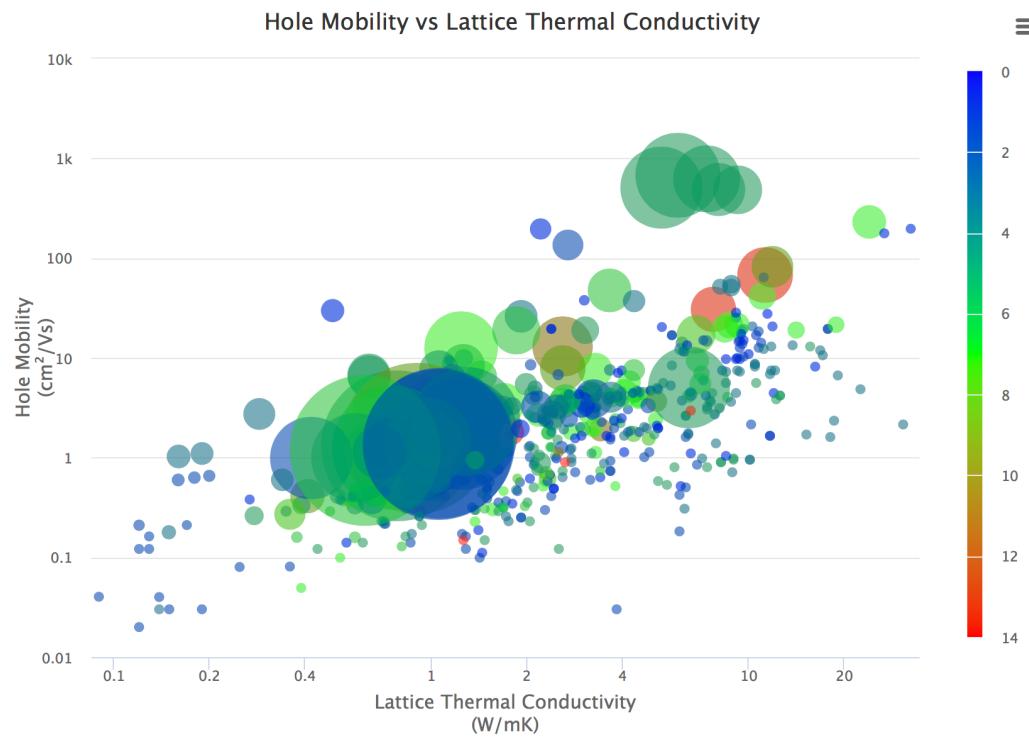
Density  
Volume  
Band Gap (DFT)  
Number of Atoms  
Band Degeneracy (VB)  
Band Degeneracy (CB)  
Hole Mobility  
Electron Mobility  
DOS Mass (VB)

Select X >> (Logarithmic )  
X: Lattice Thermal Conductivity

Select Y >> (Logarithmic )  
Y: Hole Mobility

Select Radius >> (None   
R:  $\beta(p)$

Select Heat >> (None   
Heat: Band Degeneracy (VB)



Number of Elements  
1 - 50

Space Group  
1 - 230

Crystal System  
Not specified

<http://www.tedesignlab.org>

# Batteries: Electrical Energy Storage

Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

**Explore Batteries**

by Elements ▾ Li-O-Fe-P- search

1 H	2 He																
3 Li	4 Be																
11 Na	12 Mg																
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57-71 La-Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89-103 Ac-Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn						

# of elements (including working ion)  
e.g., 4 or >2 & <6

excluded elements  
Cl Br

Submit

Intercalation

Conversion

Working Ion  
Any ▾

+ charged	Fe(PO <sub>3</sub> ) <sub>3</sub>	0.016	Energy Above Hull (eV/atom)	Volume Change	Capacity	Voltage
- discharged	LiFe(PO <sub>3</sub> ) <sub>3</sub>	0.004	Energy Above Hull (eV/atom)	3%	89 mAhg <sup>-1</sup>	3.60 V

# Photovoltaics: Light to Electricity

molecular  
space

Home    Participate ▾    Explore ▾    Design    News    FAQs ▾    About Us ▾

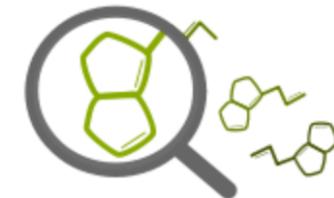
## Explore

Welcome to the Clean Energy Project Database: an Information Hub for Organic Electronics

Access the CEPDB

The **Clean Energy Project Database** (CEPDB) is a massive reference database for organic semiconductors with a particular emphasis on photovoltaic applications. It was created to store and provide access to data from computational as well as experimental studies, on both known and virtual compounds. It is a free and open resource designed to support researchers in the field of organic electronics in their scientific pursuits.

The CEPDB was established as part of the **Harvard Clean Energy Project** (CEP), a virtual high-throughput screening initiative to identify promising new candidates for the next generation of carbon-based solar cell materials. It is maintained by the **Aspuru-Guzik Research Group** in the Department of Chemistry and Chemical Biology at **Harvard University** and supported by a number of external partners. The bulk of the computational data was generated in collaboration with IBM's **World Community Grid**, a virtual supercomputer that harnesses surplus computing power donated by hundreds of thousands of volunteers around the world.



# Summary – Key Points

---

- First-principles materials modelling is increasingly powerful and predictive
- Care must be taken to choose the best method for the problem
- Materials data is increasingly important and is emerging as a new field of research with many possibilities