

Yonsei University Graduate Class

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

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Department of Materials
Imperial College London



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



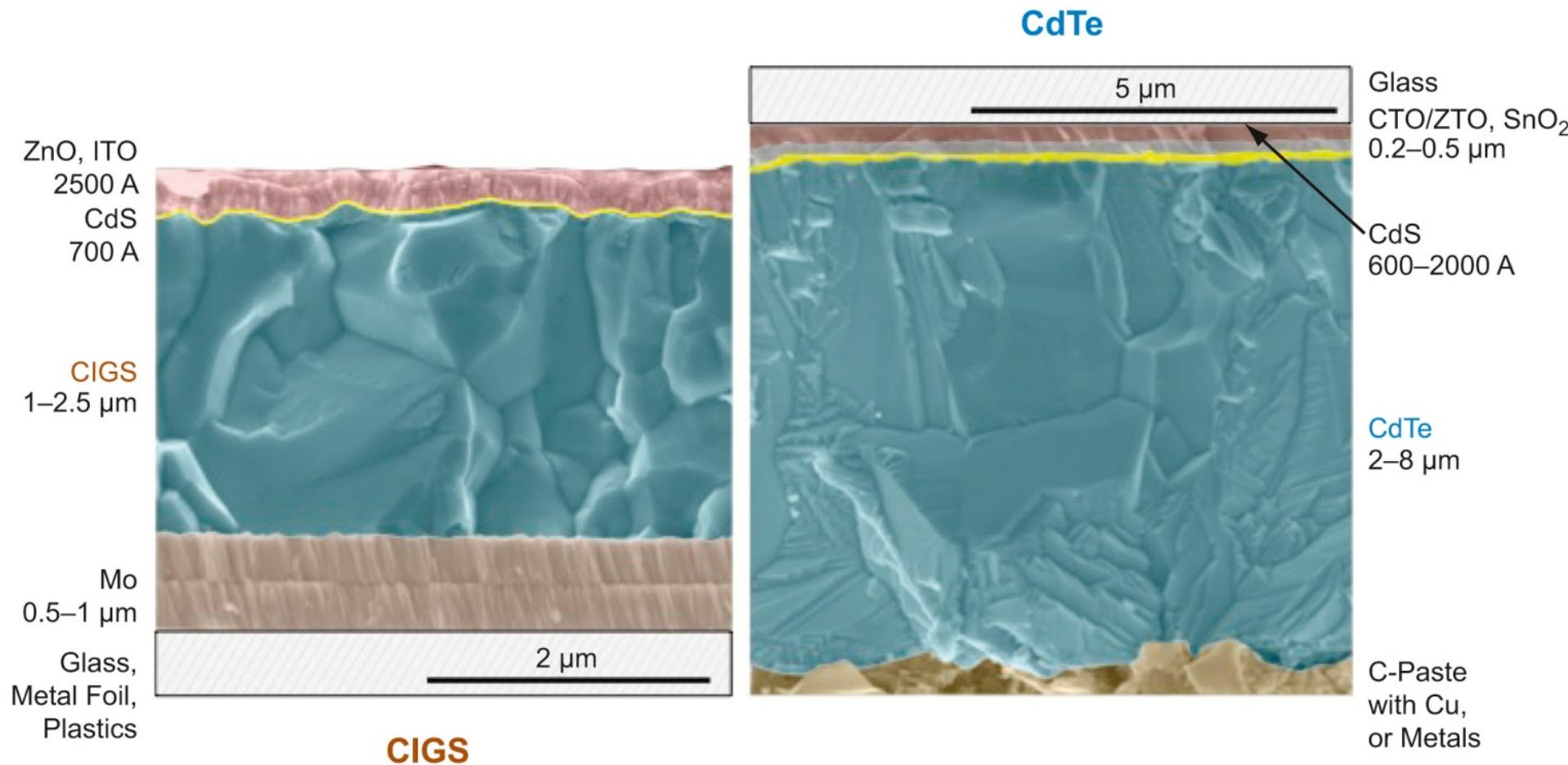
@lonepair

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

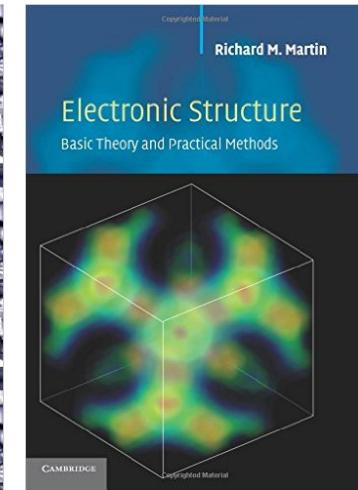
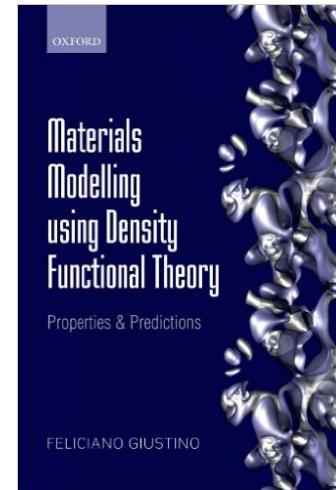
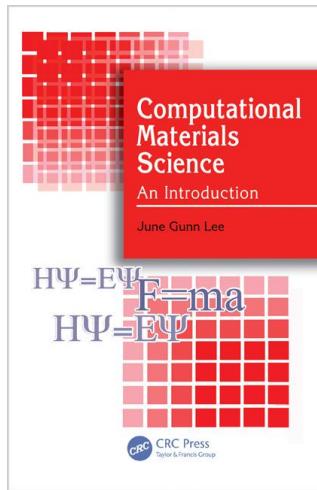
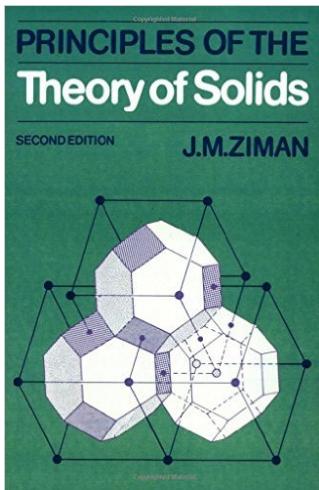
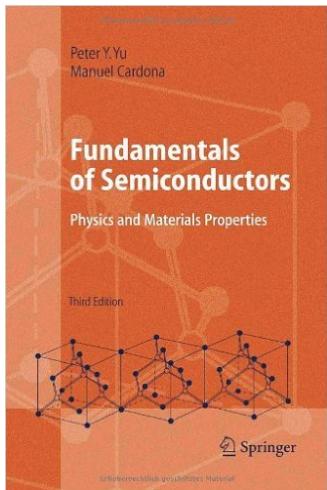
Active Layer

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

Back Contact

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

Relevant Textbooks



General

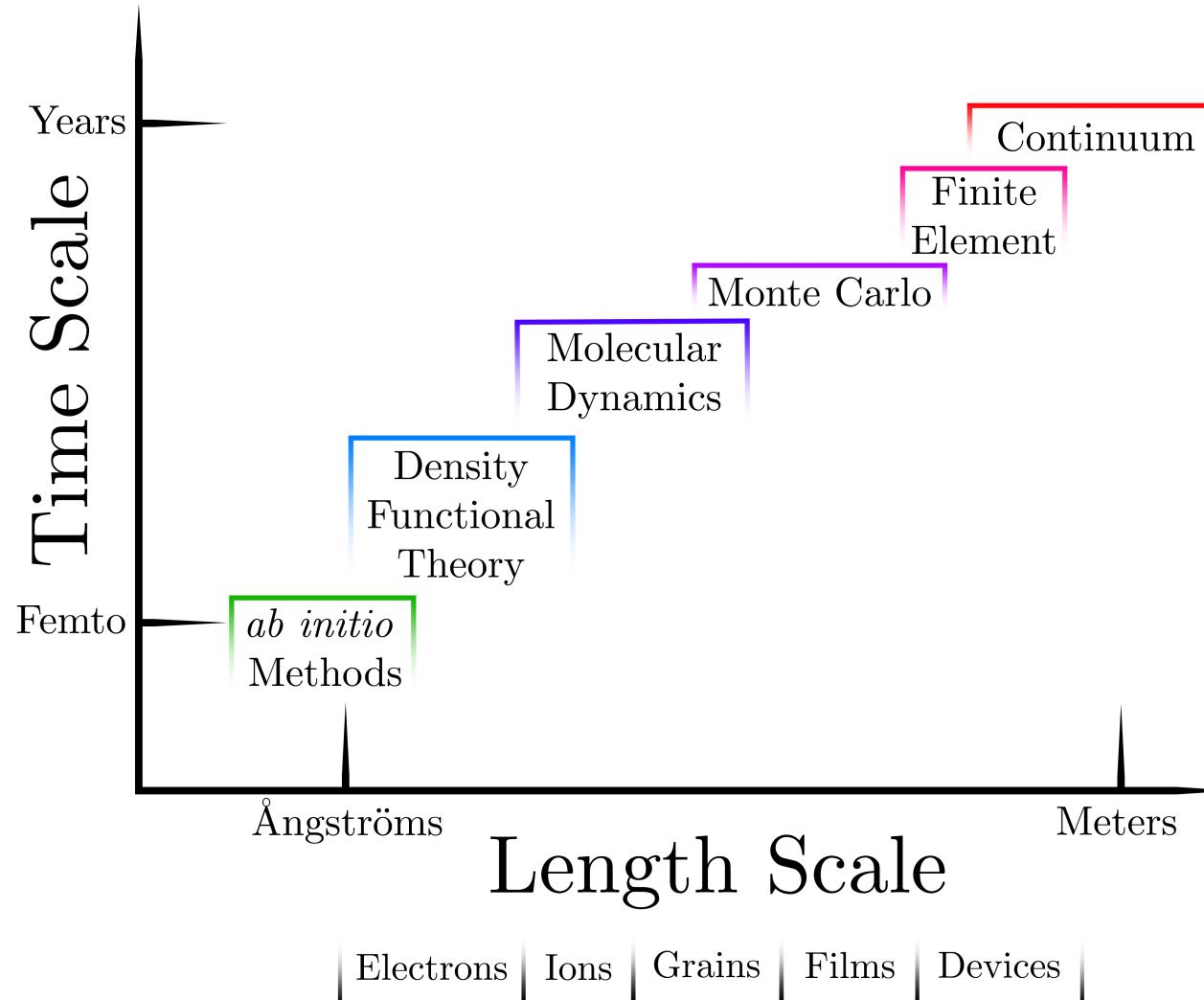
Specialist



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

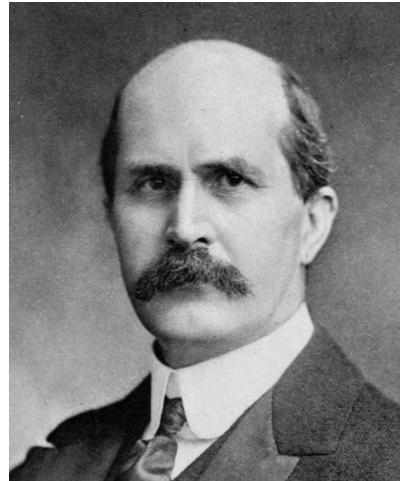
First-Principles Workflow

Input:
Structure



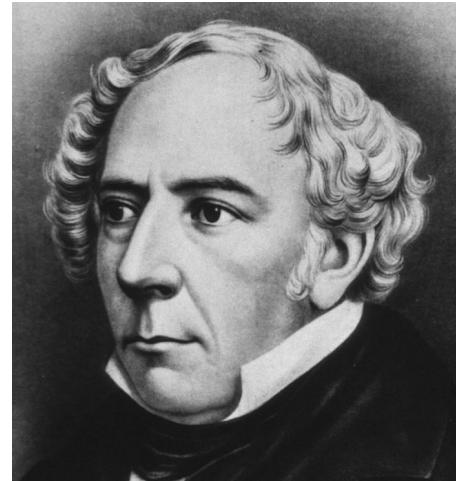
Output:
Properties

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

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

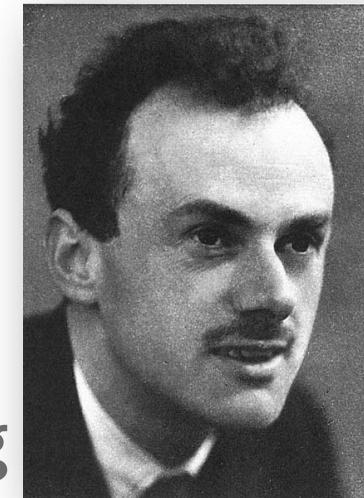
Non Relativistic

Relativistic



Schrödinger
(1887, Vienna)

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



Electronic Structure Techniques

Wavefunction
based quantum
mechanics

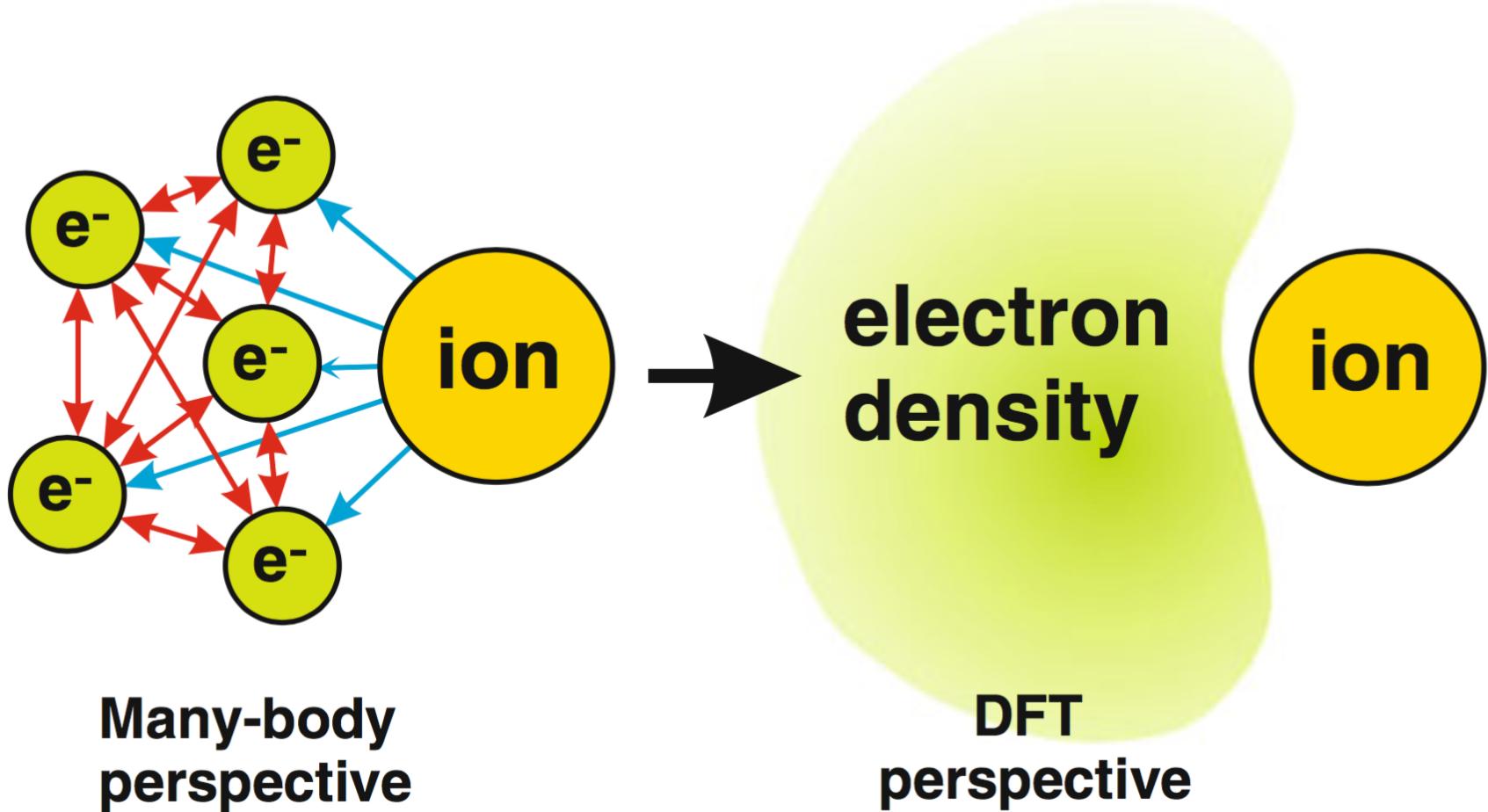
Density based
quantum
mechanics

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

Methods
Hartree-Fock
Møller-Plesset
Configuration Interaction

Methods
Thomas-Fermi
Density Functional
Dynamical Mean Field

Density Functional Theory (DFT)



Kohn-Sham DFT (1965)

Use one-electron Ψ_i that reproduce interacting ρ

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

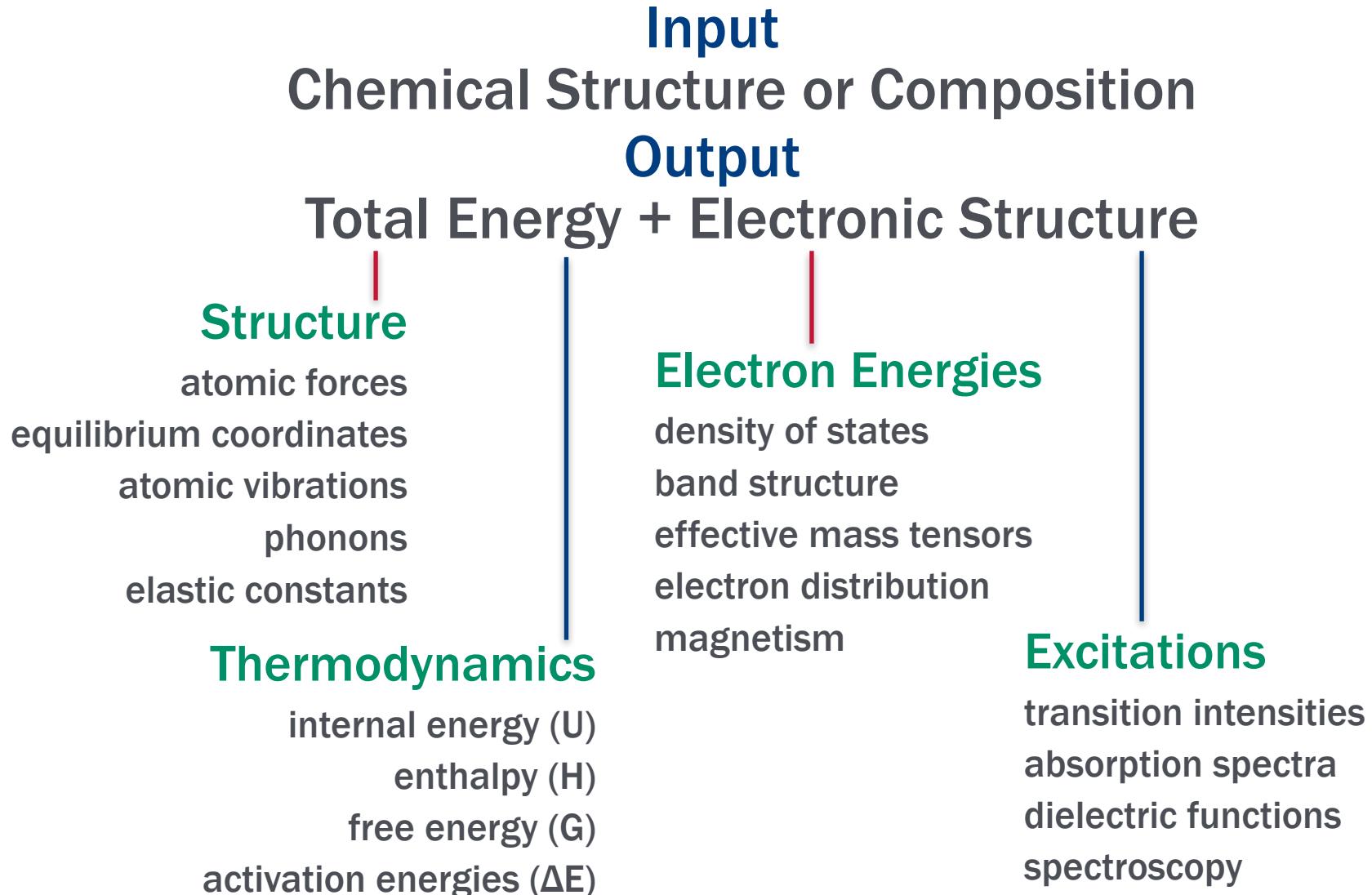
restricted
unrestricted
non-collinear

QMC
GW
RPA
TD-DFT

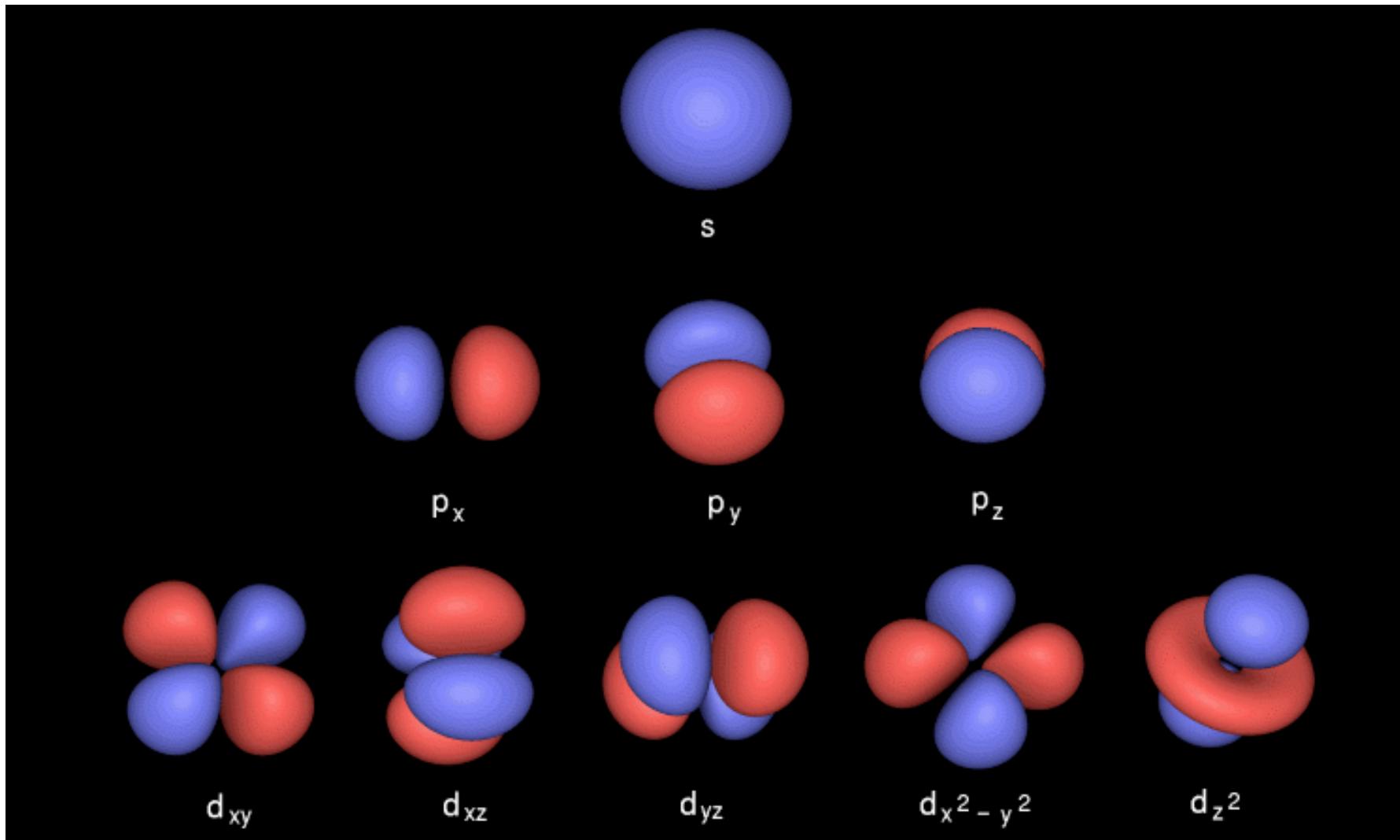
Basis Set

plane waves
numerical orbitals
analytical functions

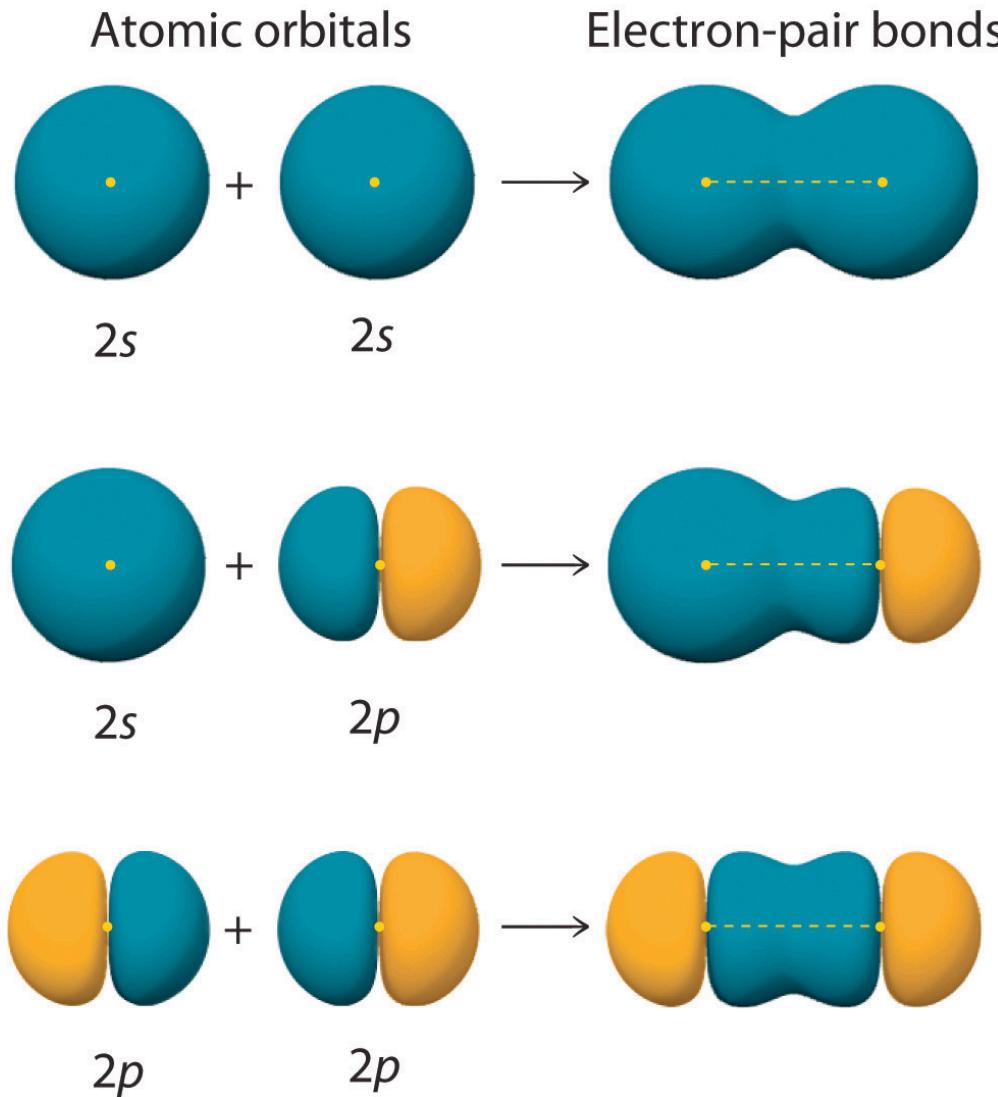
Materials Modelling with DFT



Exact (Analytical) Wavefunctions

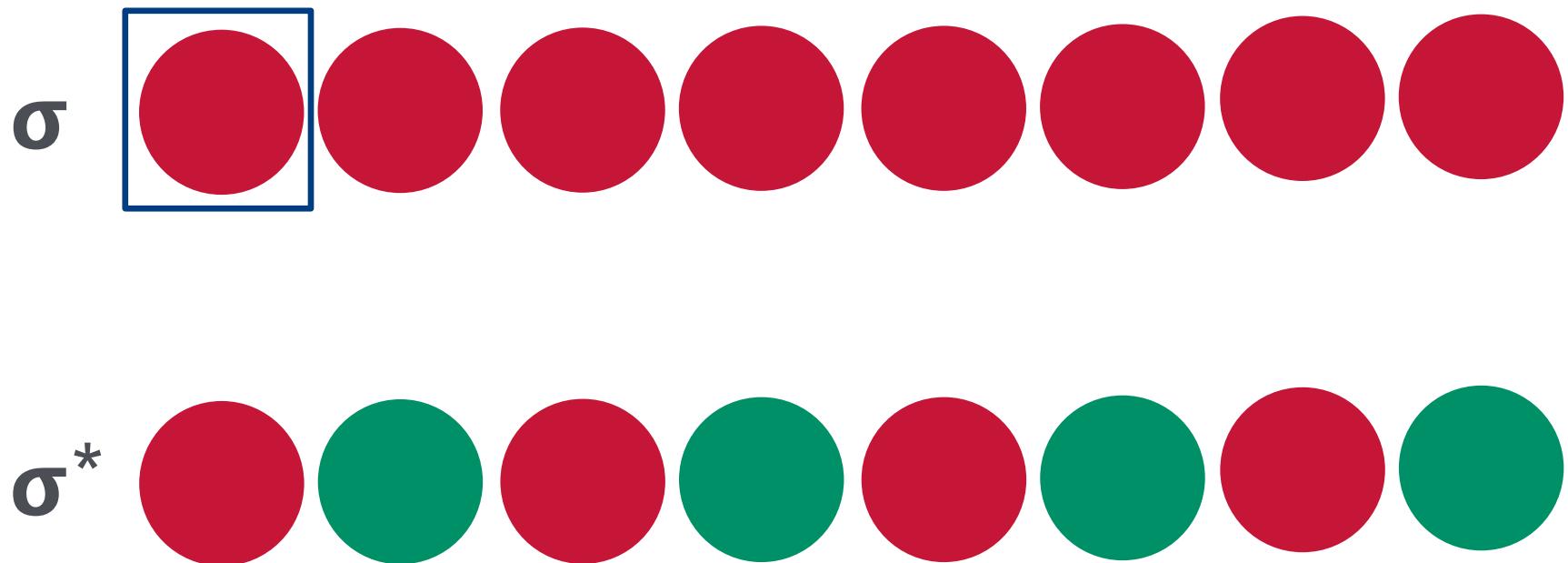


From Atoms to Molecules

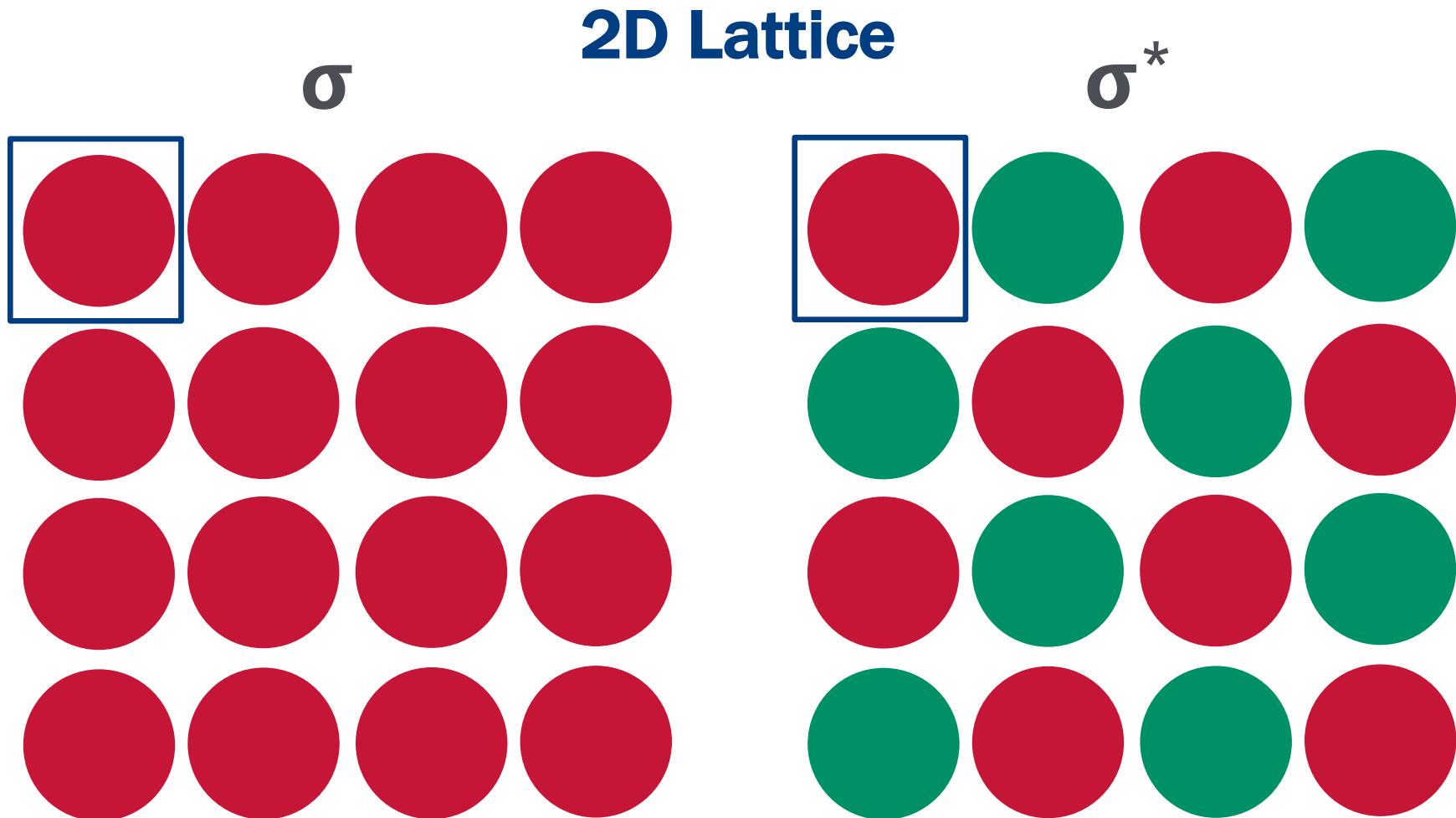


From Molecules to 1D Chain

1D Chain of Atoms



From 1D Chain to 2D Lattice



Class Question

How to combine description
of short-range (within a unit
cell) and long-range (between
unit cells)?

3D Periodic Boundary Conditions

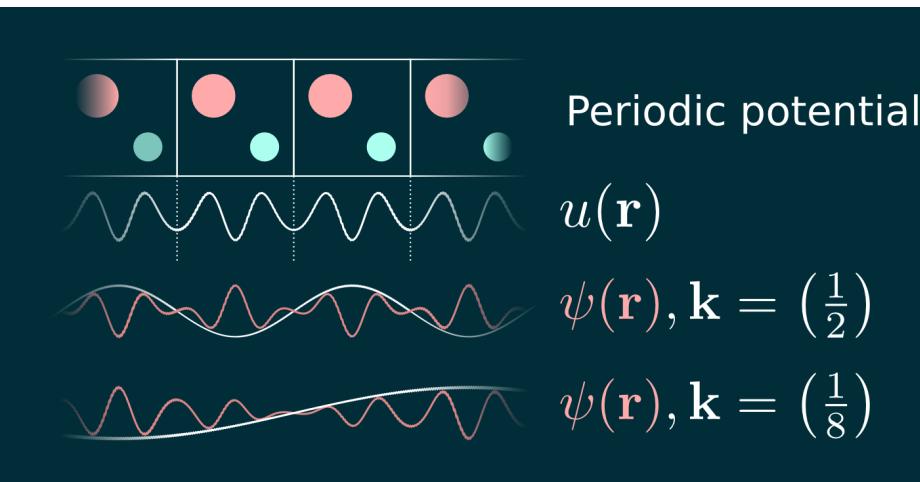
Felix Bloch (1928)

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

Crystal wavefunction

Periodic cell
potential

Plane wave



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

Electron wavevector
or
Electron momentum

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](#)

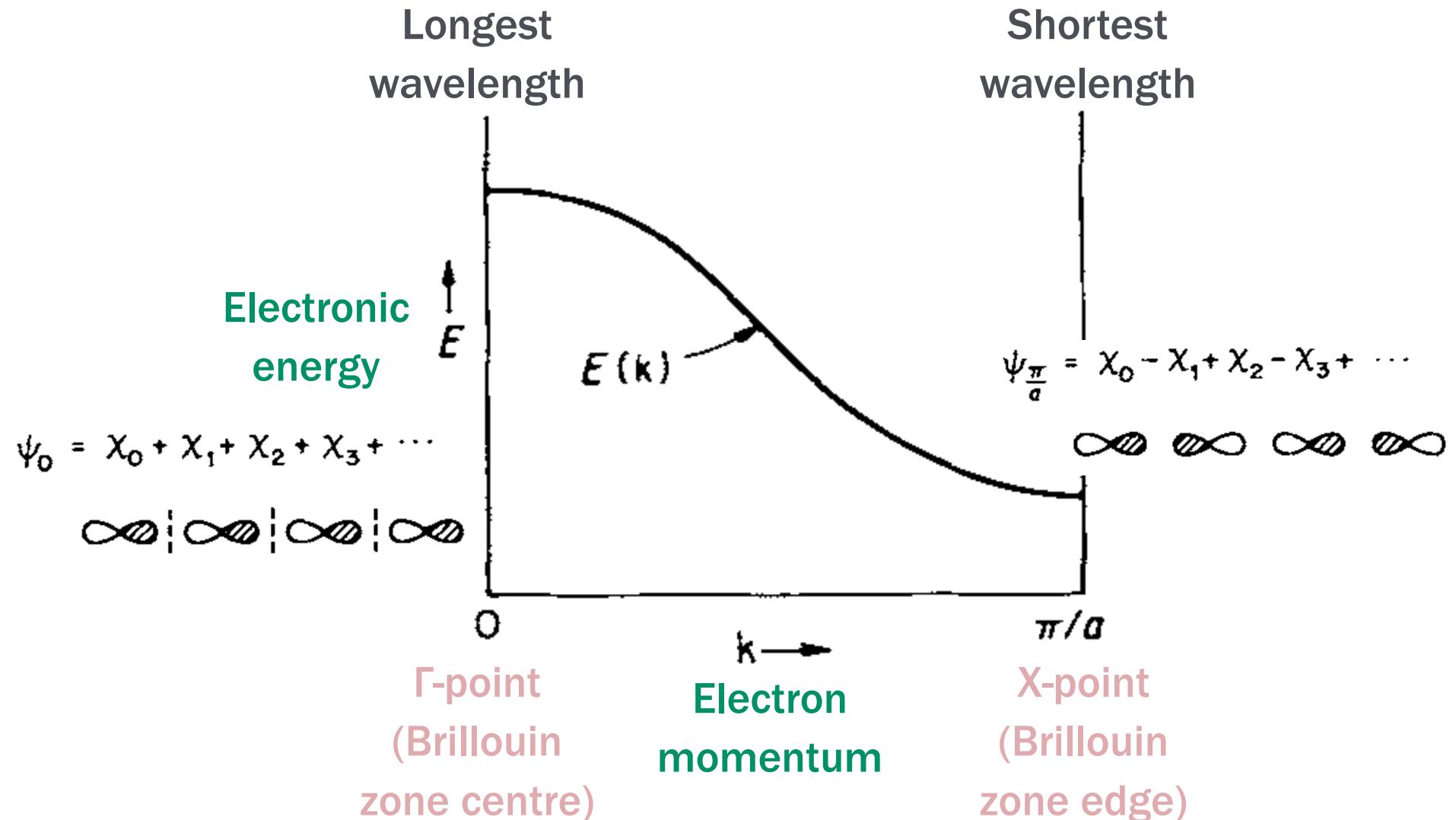


[View issue TOC](#)
Volume 26, Issue 9
September 1987
Pages 846–878

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.

How to Read a Band Structure



Band Structure: Si

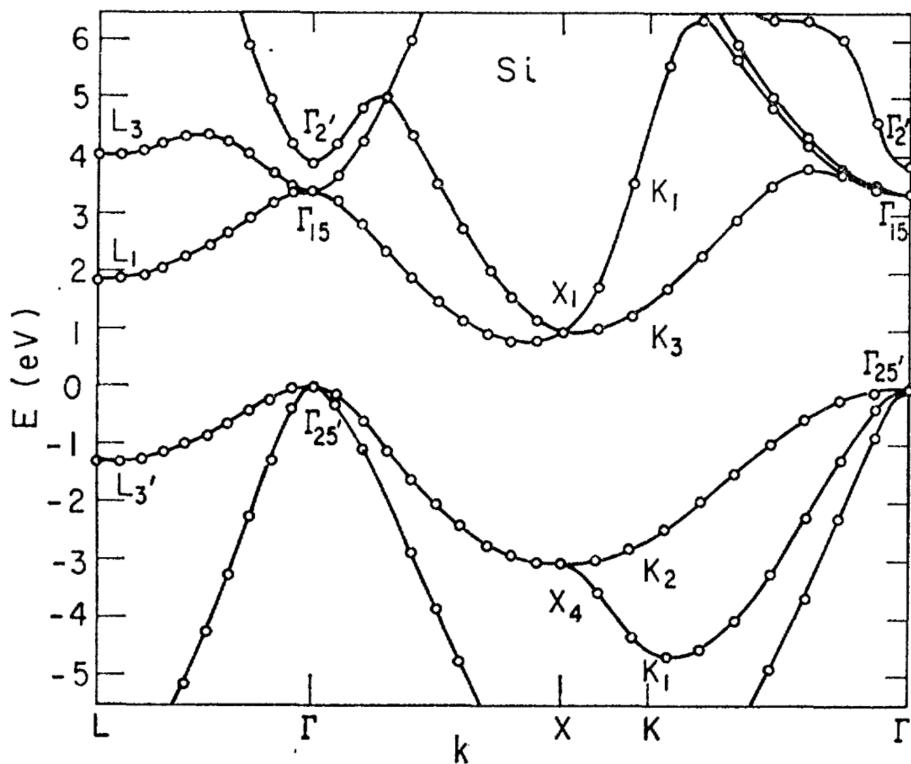
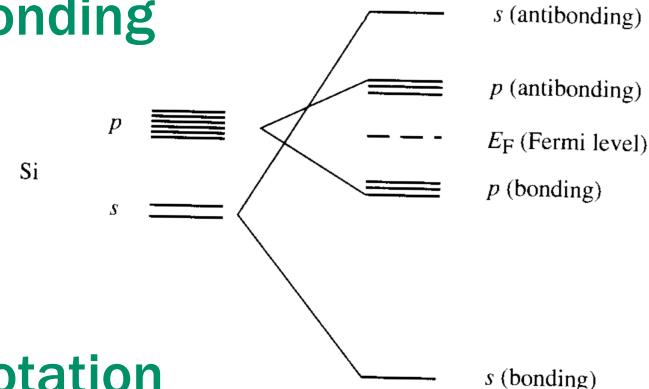


FIG. 1. Band structure of Si.

Empirical Pseudopotential Approach
Physical Review 141, 789 (1966)

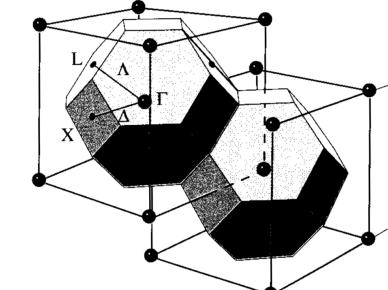
Bonding



Notation

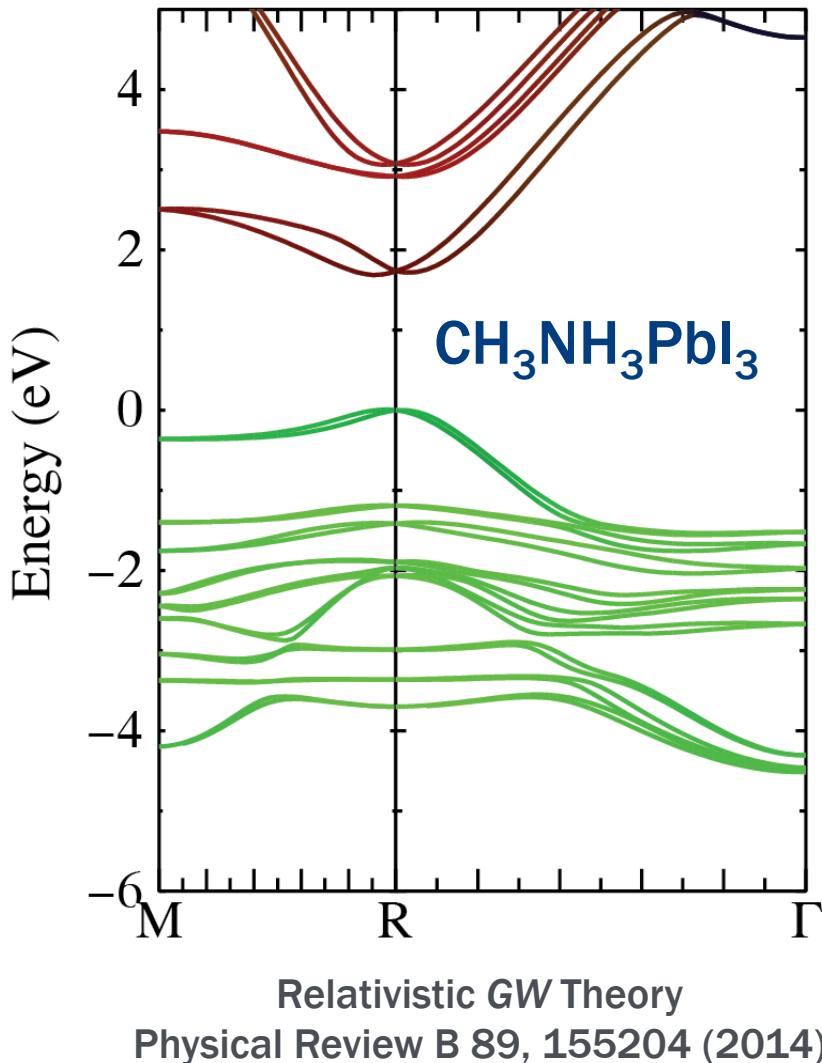
Koster notation	BSW notation	Molecular notation
Γ_1	Γ_1	A_1
Γ_2	Γ_2	A_2
Γ_3	Γ_{12}	E
Γ_4	Γ_{15}	T_2
Γ_5	Γ_{25}	T_1

Brillouin Zone

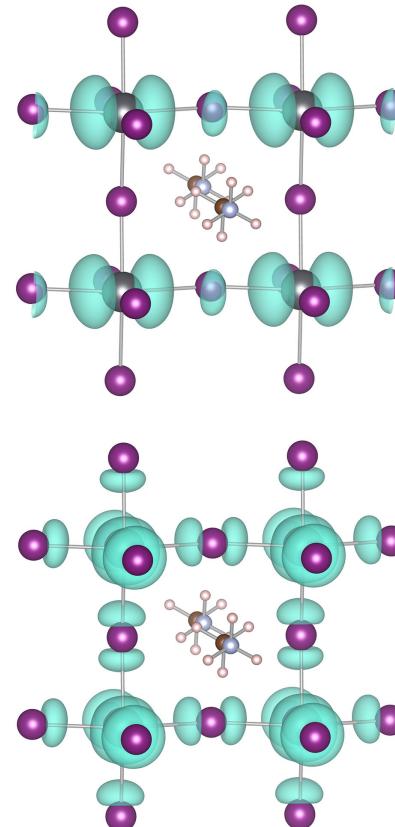


Fundamentals of Semiconductors
Yu and Cardona (Springer, 1995)

Band Structure: Perovskite



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



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	Sunway TaihuLight - 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	Tianhe-2 (MilkyWay-2) - 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	Titan - 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	Sequoia - 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	Cori - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect Cray Inc.	622,336	14,014.7	27,880.7	3,939

Probe Materials Chemistry and Physics

**Understanding known compounds
and designing new materials**

Materials Characterisation

Bulk physical and chemical properties

Chemical Reactions

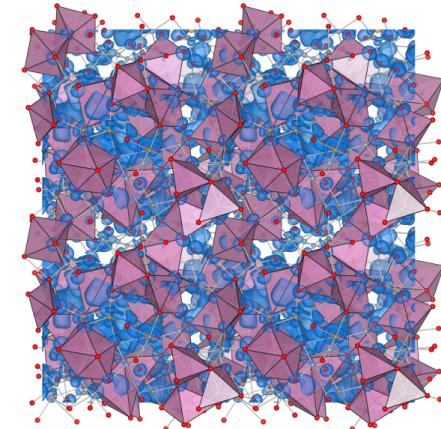
Catalysis; lattice defects; redox chemistry

Materials Engineering

Beneficial dopants, alloys, or morphology

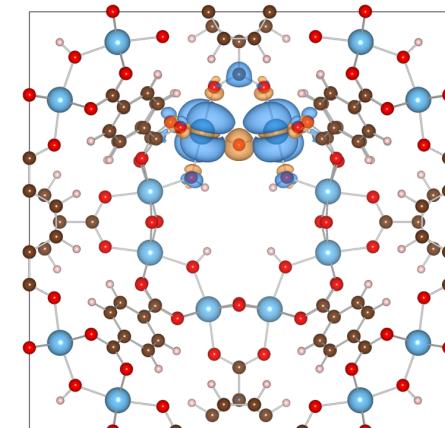
Substrate & Device Effects

Interfacial & strain phenomena



Amorphisation

Conduction states in InGaZnO_4



Hybrid Network

Photochromic MIL-125

Same Method – Same Result

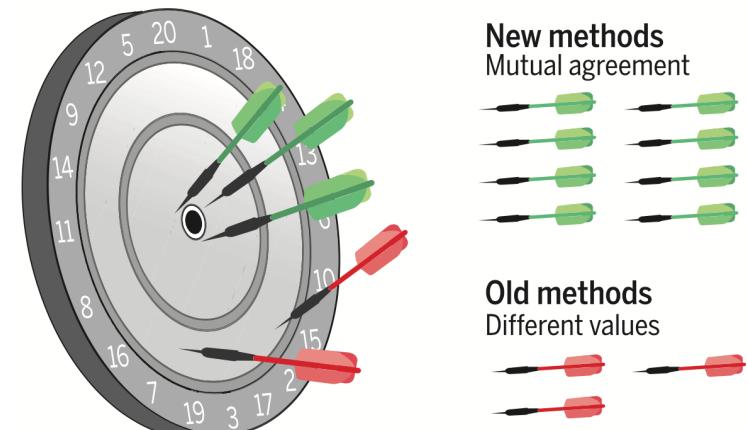
RESEARCH ARTICLE

DFT METHODS

Reproducibility in density functional theory calculations of solids

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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

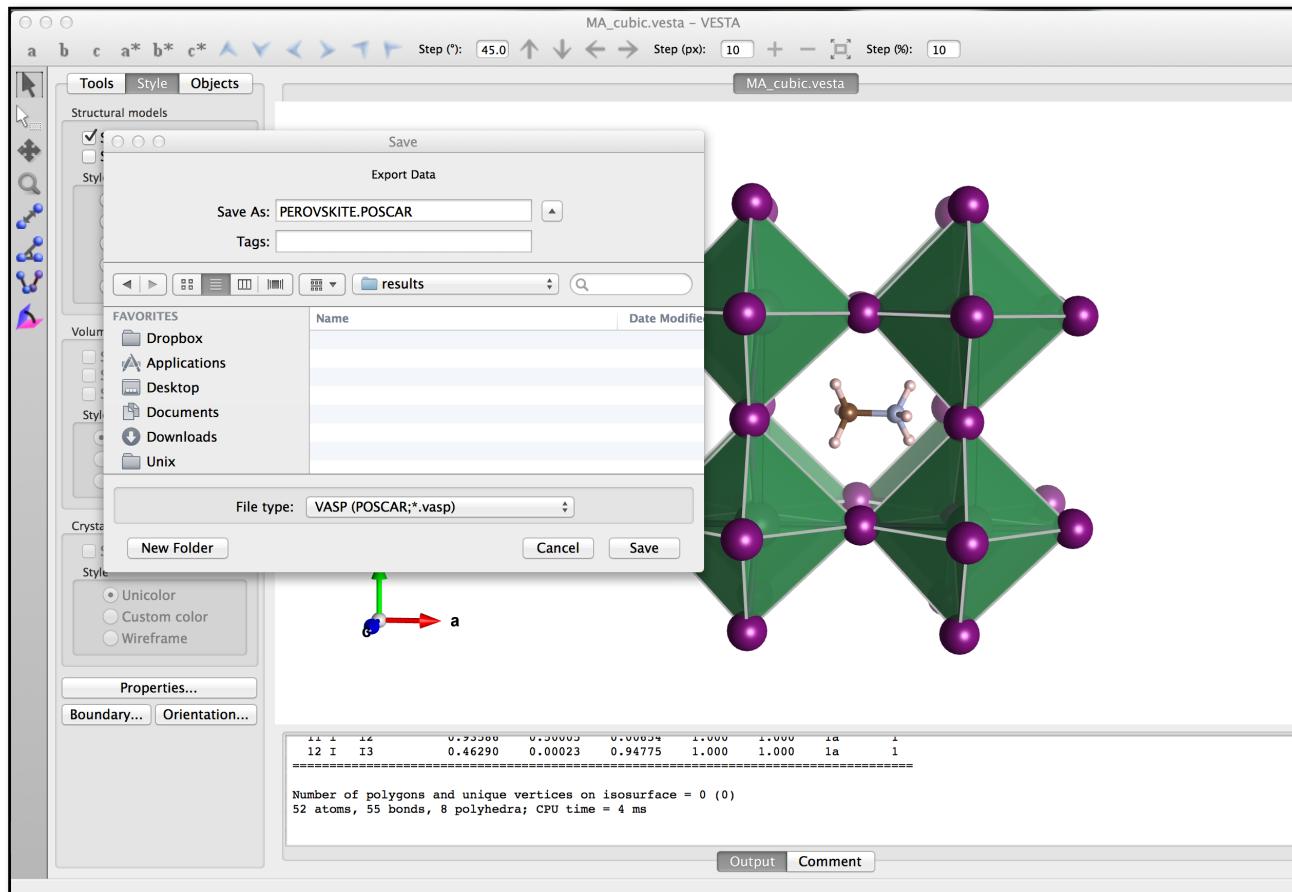
- **OUTCAR** (“Output Card”)
- **CONTCAR** (“Continue [Positions] Card”)
- **CHGCAR** (“Charge Density Card”)
- **vasprun.xml** (Auxiliary output as xml)

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
```

!Ionic Relaxation:	INCAR (Partial)
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	KPOINTS
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
β -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

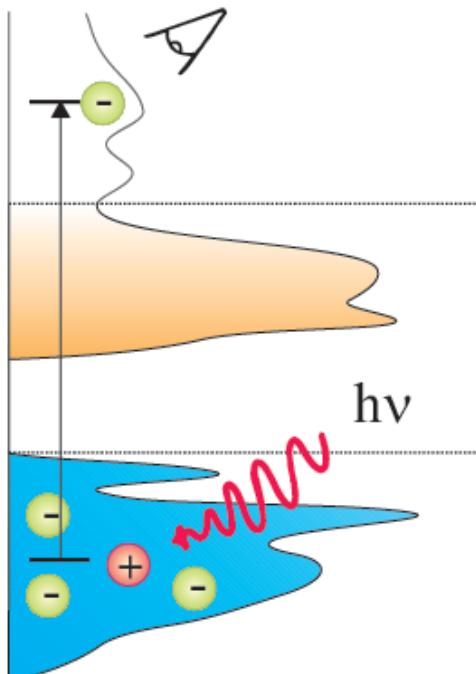
Recommended: PBEsol (GGA for solids) & HSE06 (screened hybrid GGA)

Journal of Chemical Physics 123, 174101 (2005)

Electronic Spectroscopy

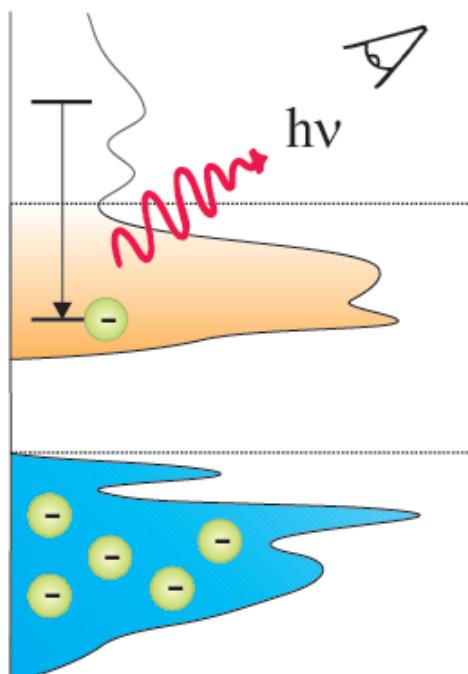
Electronic band gap \neq Optical band gap

Photoemission



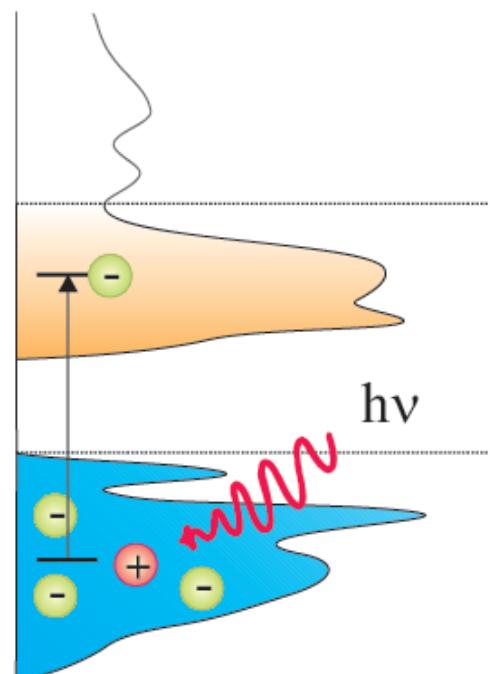
N-1 quasi-particle
(electron + interaction with environment)

Inverse Photoemission



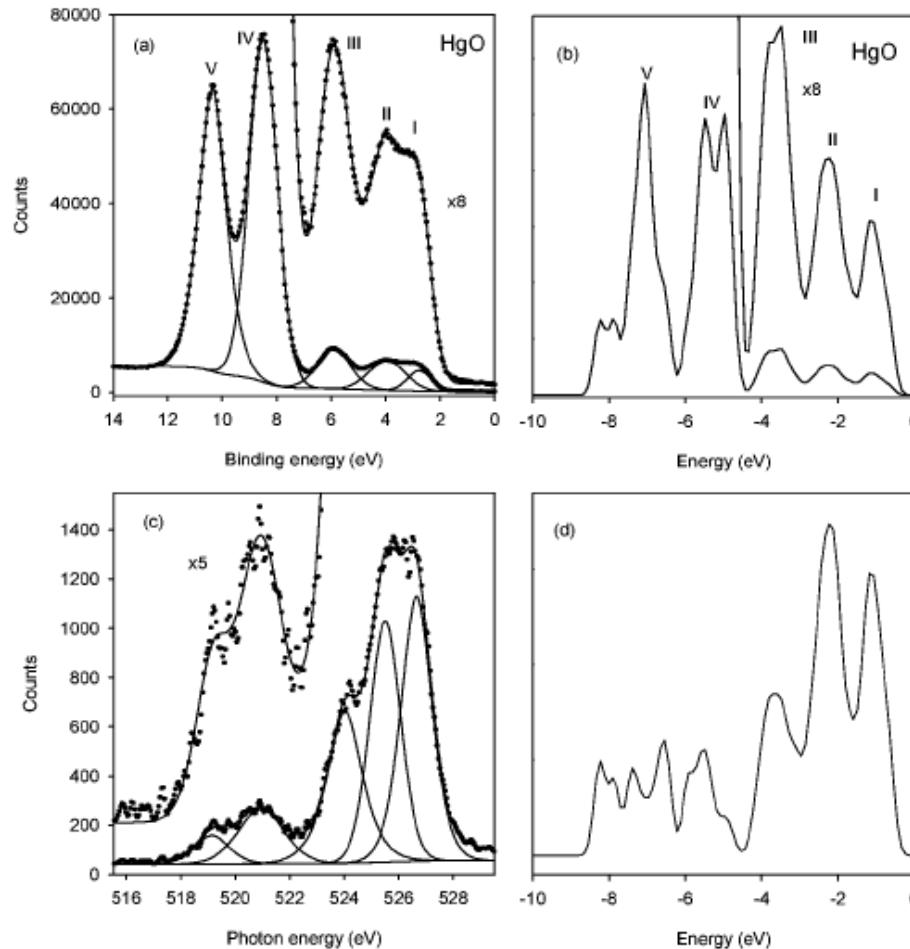
N+1 quasi-particle

Absorption



N excitation
(e-h interaction)

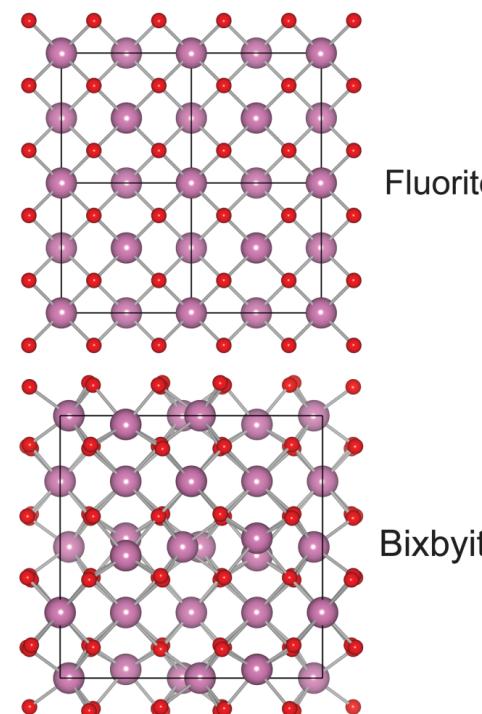
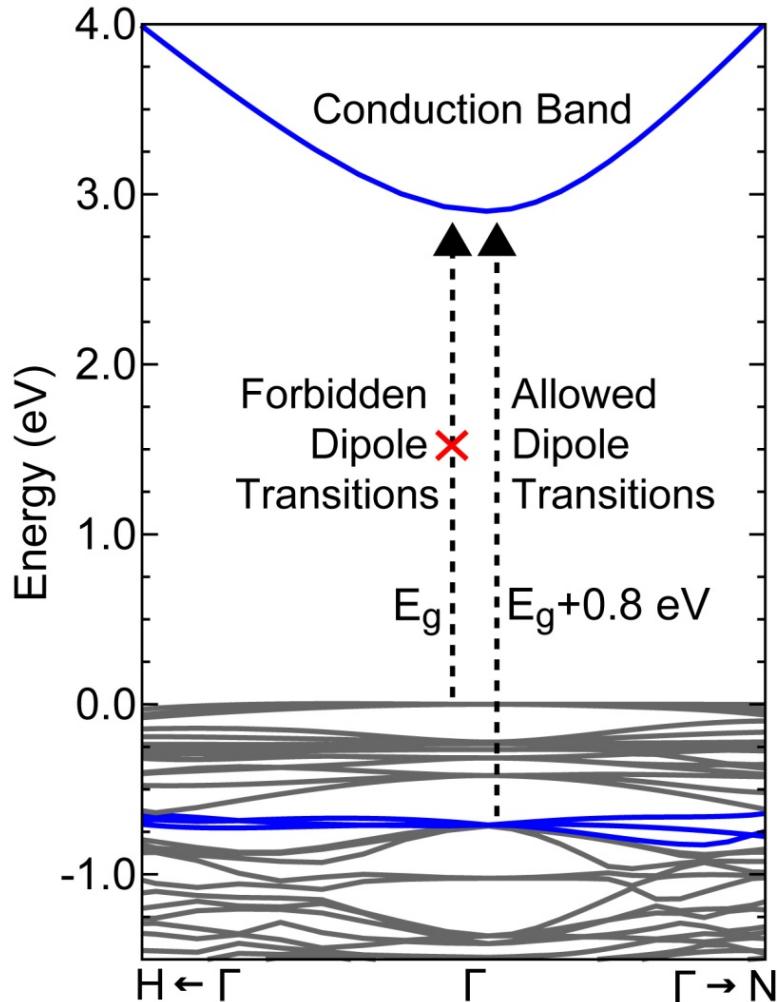
Electronic Spectroscopy: HgO



XPS
(weighted DOS)

O K XES
(O 2p DOS)

Electronic vs Optical: In_2O_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

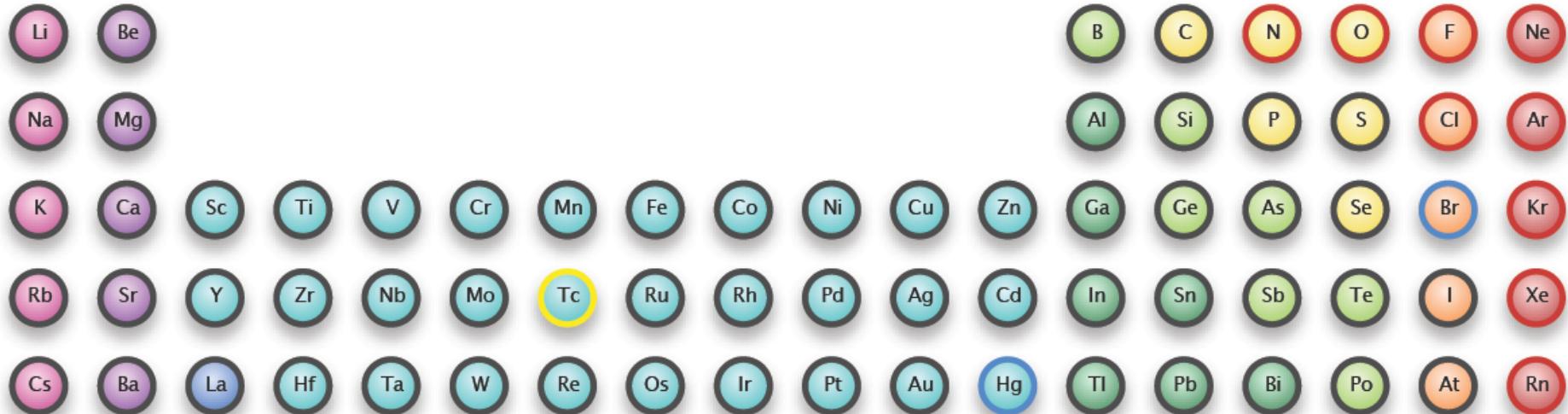
INPUT

Property

OUTPUT

Composition
Structure

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

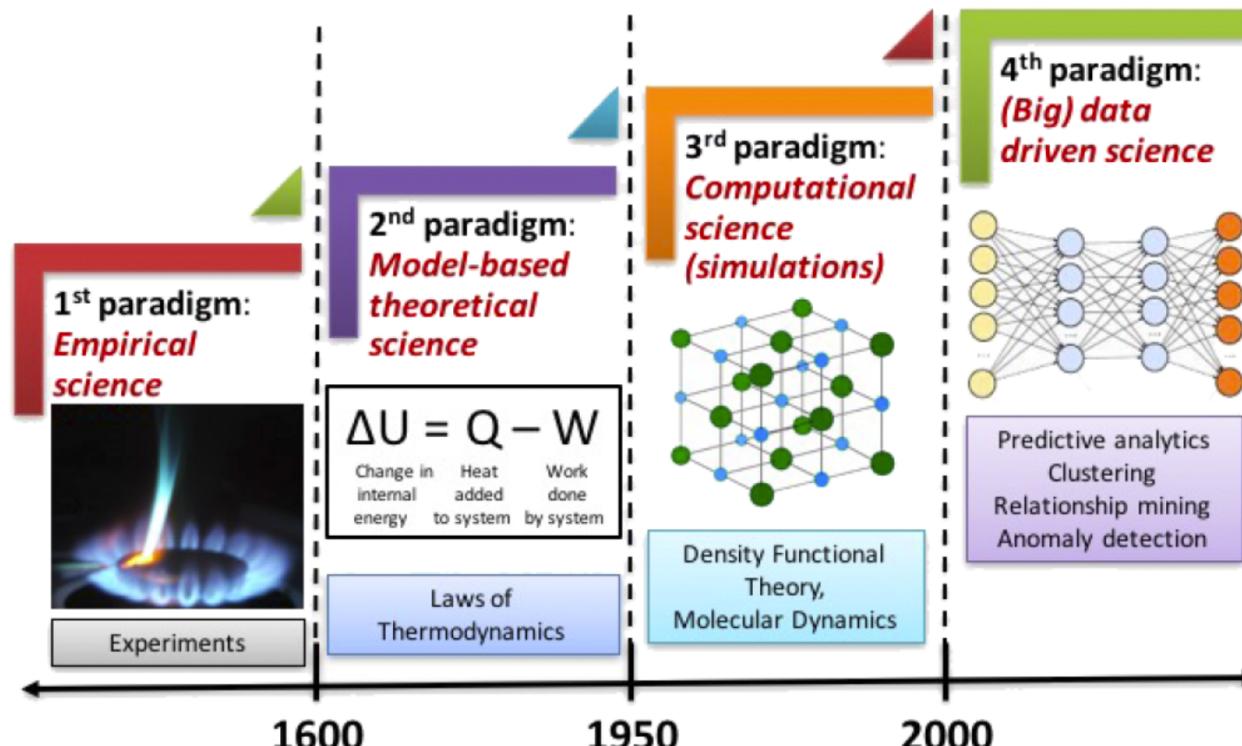
Computational Materials Design

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

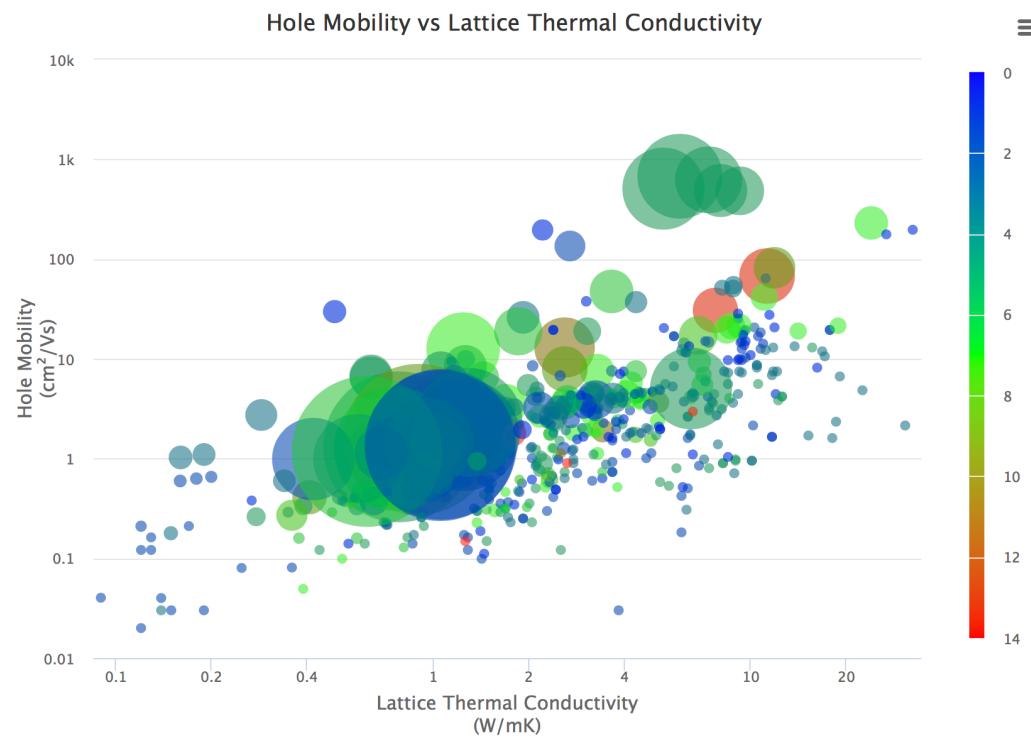
Density
Volume
Band Gap (DFT)
Number of Atoms
Band Degeneracy (VB)
Band Degeneracy (CB)
Hole Mobility
Electron Mobility
DOS Mass (VB)

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 ₃) ₃	0.016	Energy Above Hull (eV/atom)	Volume Change	Capacity	Voltage
- discharged	LiFe(PO ₃) ₃	0.004	Energy Above Hull (eV/atom)	3%	89 mAhg ⁻¹	3.60 V

Photovoltaics: Light to Electricity

molecular
space

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

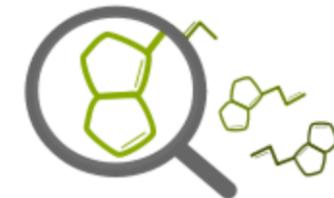
Explore

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