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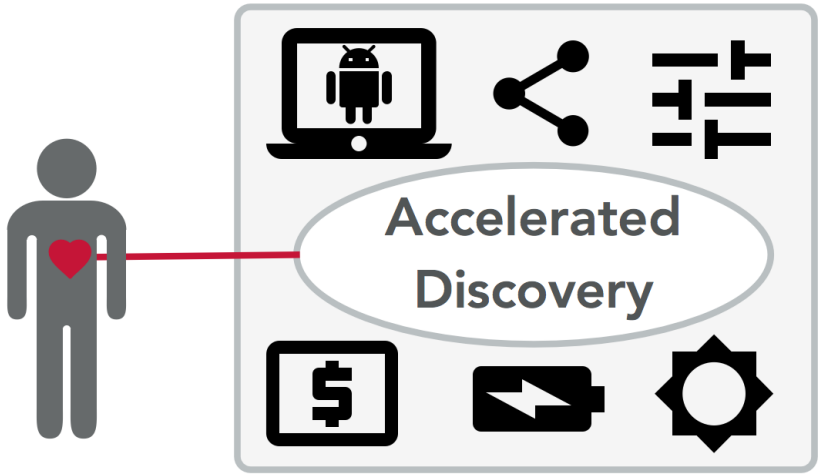
From Atoms to Devices:
Materials design for new energy technologies

Prof. Aron Walsh

Department of Materials

Imperial College London, UK



https://wmd-group.github.io @lonepair

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Chemistry to Physics to Materials

Trinity College Dublin, Ireland
BA and PhD in Computational Chemistry

National Renewable Energy Laboratory, USA
Postdoc in Materials Physics (w/ Su-Huai Wei)

University College London, UK
Marie Curie Research Fellow (w/ Richard Catlow)

University of Bath, UK
Royal Society University Research Fellow

Imperial College London, UK
Professor in Materials Design

Imperial College London

Chemistry to Physics to Materials

Trinity College Dublin, Ireland

Structure-property relationships in metal oxides

National Renewable Energy Laboratory, USA

Photovoltaics and photoelectrochemistry

University College London, UK

Electroactive metal-organic frameworks

University of Bath, UK

Kesterite and perovskite solar cells

Imperial College London, UK

Theory of imperfect crystals

Imperial College London

Bath – CSCT CDT Students

Dr. Lee Burton

SnS solar cells – PDRA at U.C. de Louvain

Dr. Adam Jackson

Thermodynamics of Cu_2ZnSnS_4– PDRA at UCL

Dr. Jessica Bristow

Metal-organic frameworks – PDRA at Liverpool

Suzanne Wallace

Defects in metal sulfide solar cells

Daniel Davies

Materials screening and informatics

Imperial College London

ICL – Department of Materials

Imperial College London

Thomas Young Centre

Theory and Simulation of Materials:

Seminars, Workshops, Networking, and Outreach

Coverage in Nature Materials 15, 371 (2016)

Connects 100 Research Groups:

- Imperial College London
- University College London
- Kings College London
- Queen Mary University

http://www.thomasyoungcentre.org

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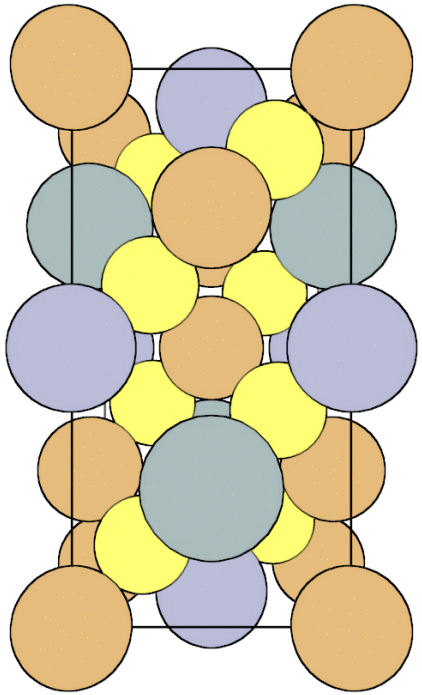
Solar Minerology

Developing sustainable energy technologies: from minerals to devices

Kesterite Mineral



Cu_2ZnSnS_4

Solar Panel

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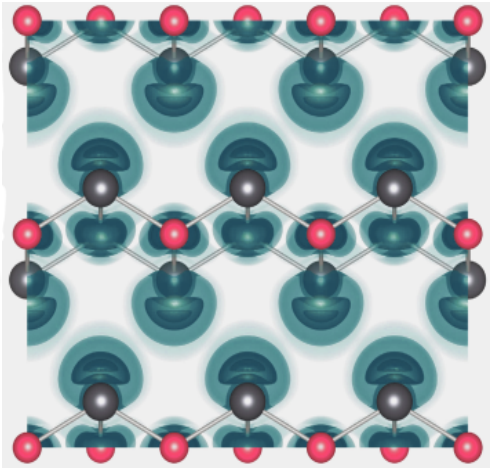
Transparent Electronics

Compounds that conduct electricity and are optically transparent

Copper Wire



IGZO
($In_xGa_yZn_zO$)

HD-TFT Displays

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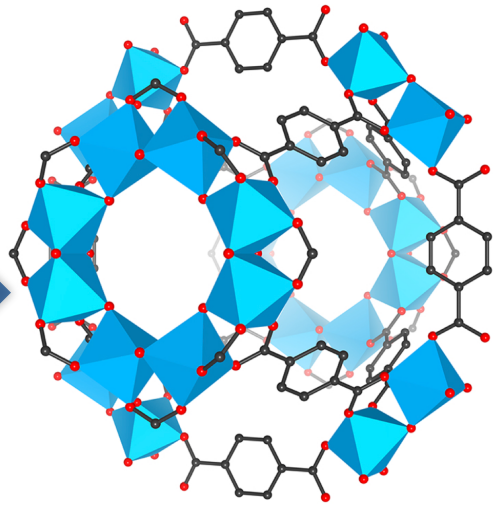
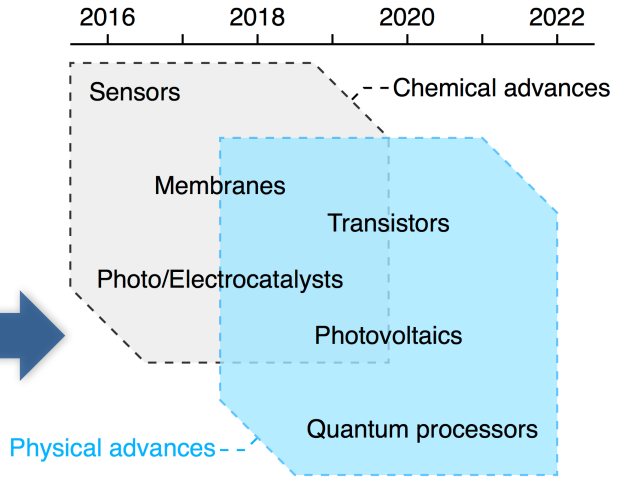
Metal-Organic Frameworks (MOFs)

Functional porous crystals from organic and inorganic building blocks

Molecular Self-assembly



MIL-125



Technology Roadmap

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Talk Motivation

New Materials for Energy Technologies

- Performance
- Cost
- Stability
- Sustainability

Is computational materials design now a reality?

Imperial College London

Talk Outline

1. Materials Modelling in 2017
2. From Atoms to Devices

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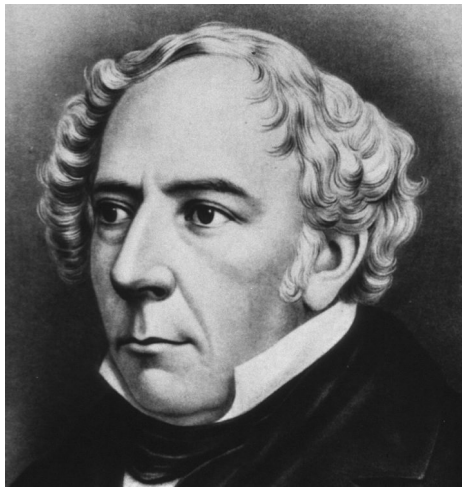
First-Principles Materials Modelling

Input: **Structure** → **Output:** **Properties**

X-ray Diffraction	Hamiltonian	Physical Chemistry
(unit cells)	(ions and electrons)	(stimuli)
		
Kathleen Lonsdale *(Kildare, 1903)*	William Hamilton *(Dublin, 1805)*	Robert Boyle *(Waterford, 1627)*

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Equations too Difficult to Solve

Relativistic Quantum Mechanics

$$(i\partial\!\!\!/ - m)\Psi = 0$$

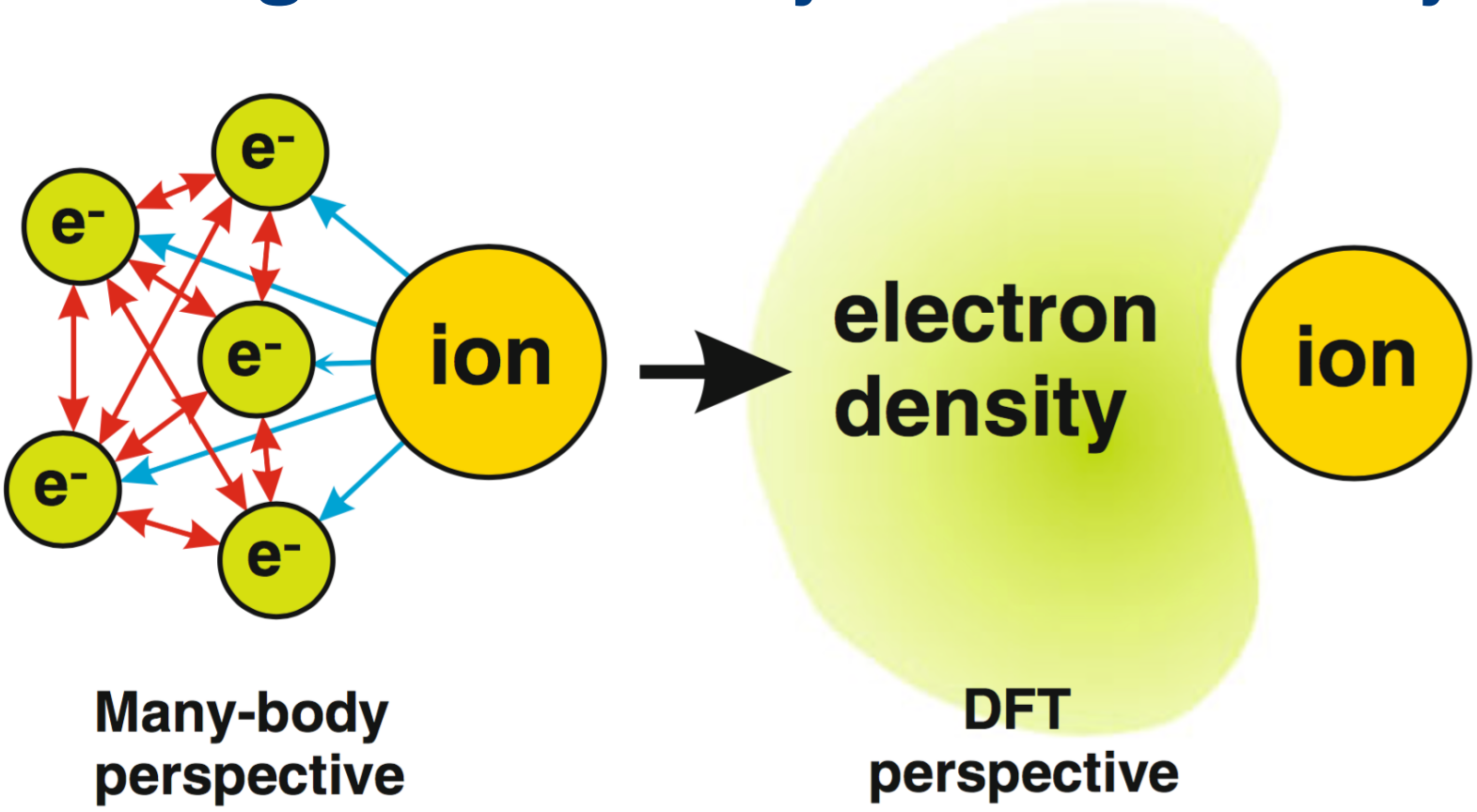
The Dirac equation doesn't look too difficult, but here it is in a heavily condensed form (thanks to Feynman slash notation and tricks from geometric algebra)

"Approximate practical methods of applying quantum mechanics should be developed"

Paul Dirac, 1929

Approximate Theories

Emergence of Density Functional Theory



Source: F. Bechstedt – Many-body Approach to Electronic Excitations (2015)

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2017 Supercomputers (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

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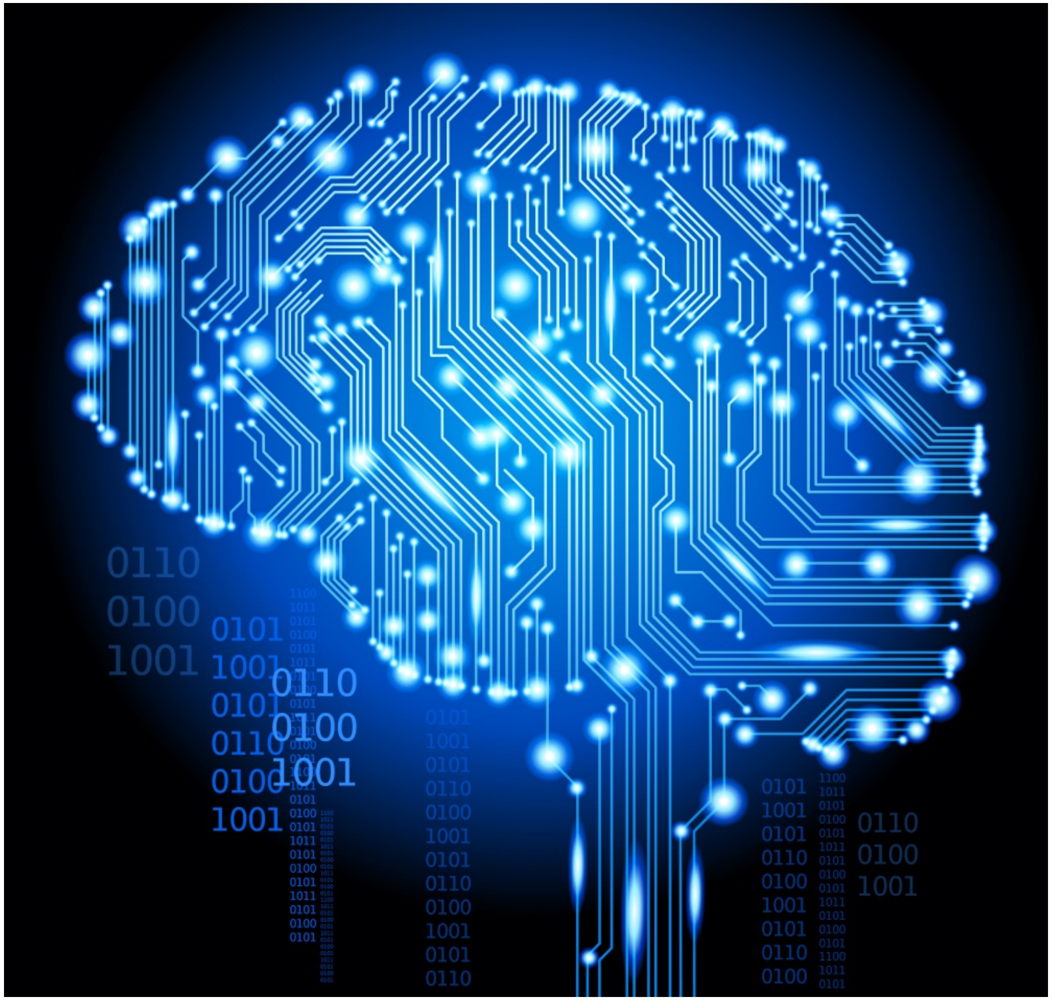
Exascale Computing (10^{18} FLOPS)



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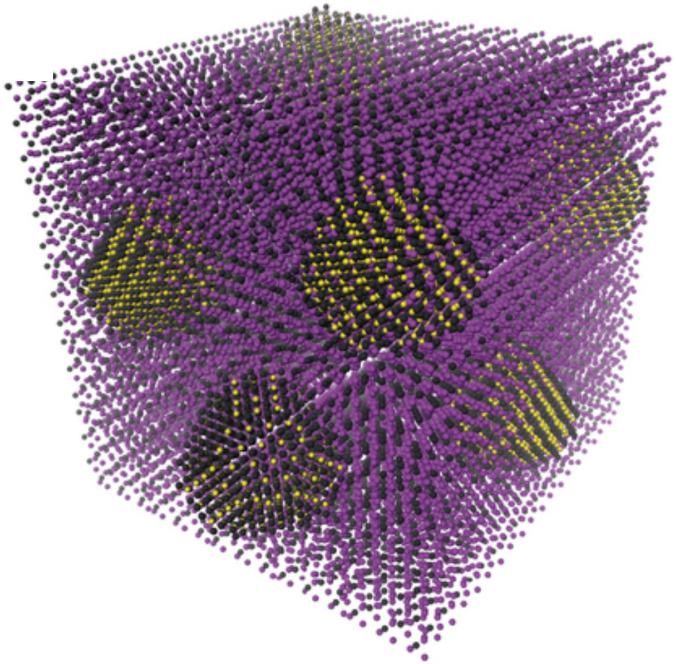
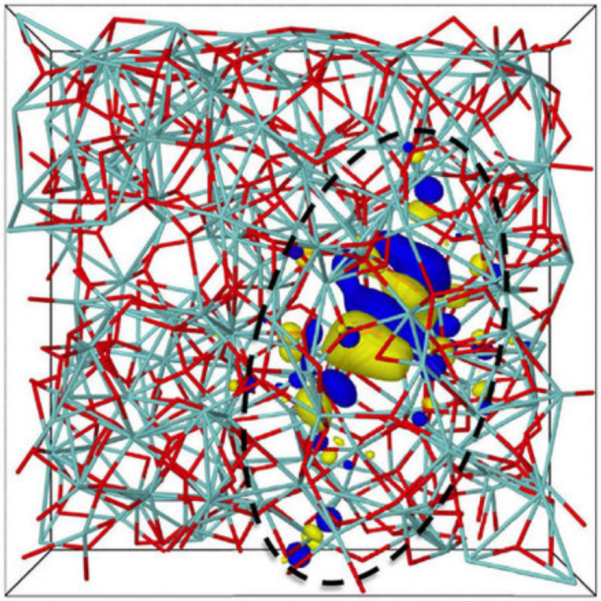
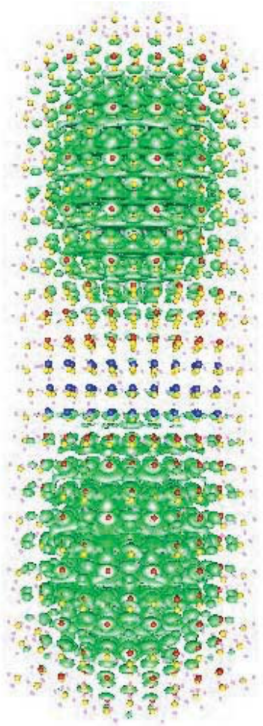
Thousands of Interacting Electrons







“With density functional theory as your hammer, everything starts to look like a nail”

Chris Pickard (University of Cambridge), 2009

Past: Local Optimisation

INPUT	OUTPUT
Structure	Properties

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Past: Local Optimisation

PHYSICAL REVIEW B VOLUME 17, NUMBER 12 15 JUNE 1978

Local-density self-consistent energy-band structure of cubic CdS

Alex Zunger* and A. J. Freeman
Department of Physics and Astronomy, and Materials Research Center, Northwestern University, Evanston, Illinois 60201
(Received 9 February 1978)

Self-consistent *ab initio* studies of the electronic-energy-band structure of cubic CdS are reported within the local-density-functional (LDF) formalism. All electrons are included using our previously reported linear-combination-of-atomic-orbitals method in a numerical basis representation. In the first set of calculations we employ the same lattice constant, exchange (only) potential, and computational parameters as were used by Stukel *et al.* in their early self-consistent orthogonalized-plane-wave (SCOPW) investigation so that a direct comparison of results can be made and the validity of the SCOPW approach for covalently bonded $4d$ systems can be assessed. In the second set of calculations, the Stukel *et al.* computational restrictions are relaxed, a more accurate lattice parameter is employed, and the Kohn-Sham exchange and the Singwi *et al.* correlation potential are used to obtain the local-density formalism solutions to the band problem, including variation of the band structure and related properties with pressure (change of lattice constant). Comparison with optical and x-ray and uv photoemission experiments for excitations of both the s-p and metal d bands in the 5–19 eV region indicate very good agreement. The direct gap at Γ is, however, found to be 0.5 eV (25%) too small, a discrepancy similar to that previously found in nonempirical studies for other heteropolar insulators (e.g., Ne and LiF). This is traced to the neglect of the different orbital relaxation at the Γ_{25} and Γ_1 band edges and to the noncancellation of the self-interaction terms characteristic of the local-density potential. Simple atomic total-energy models for these effects are shown to bring this gap into good agreement with experiment. It is concluded that a first-principles (parameter-free) exchange and correlation LDF model describes very well the main electronic-structure features of the system.

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Past: Local Optimisation

PHYSICAL REVIEW B **89**, 205203 (2014)

Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles

Jonathan M. Skelton,[1] Stephen C. Parker,[1] Atsushi Togo,[2] Isao Tanaka,[2,3] and Aron Walsh[1,*]
[1]*Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*
[2]*Elements Strategy Initiative for Structural Materials, Kyoto University, Kyoto Prefecture 606-8501, Japan*
[3]*Department of Materials Science and Engineering, Kyoto University, Kyoto Prefecture 606-8501, Japan*
(Received 12 March 2014; revised manuscript received 23 April 2014; published 15 May 2014)

The lead chalcogenides represent an important family of functional materials, in particular due to the benchmark high-temperature thermoelectric performance of PbTe. A number of recent investigations, experimental and theoretical, have aimed to gather insight into their unique lattice dynamics and electronic structure. However, the majority of first-principles modeling has been performed at fixed temperatures, and there has been no comprehensive and systematic computational study of the effect of temperature on the material properties. We report a comparative lattice-dynamics study of the temperature dependence of the properties of PbS, PbSe, and PbTe, focusing particularly on those relevant to thermoelectric performance, *viz.* phonon frequencies, lattice thermal conductivity, and electronic band structure. Calculations are performed within the quasiharmonic approximation, with the inclusion of phonon-phonon interactions from many-body perturbation theory, which are used to compute phonon lifetimes and predict the lattice thermal conductivity. The results are critically compared against experimental data and other calculations, and add insight to ongoing research on the PbX compounds in relation to the off-centering of Pb at high temperatures, which is shown to be related to phonon softening. The agreement with experiment suggests that this method could serve as a straightforward, powerful, and generally applicable means of investigating the temperature dependence of material properties from first principles.

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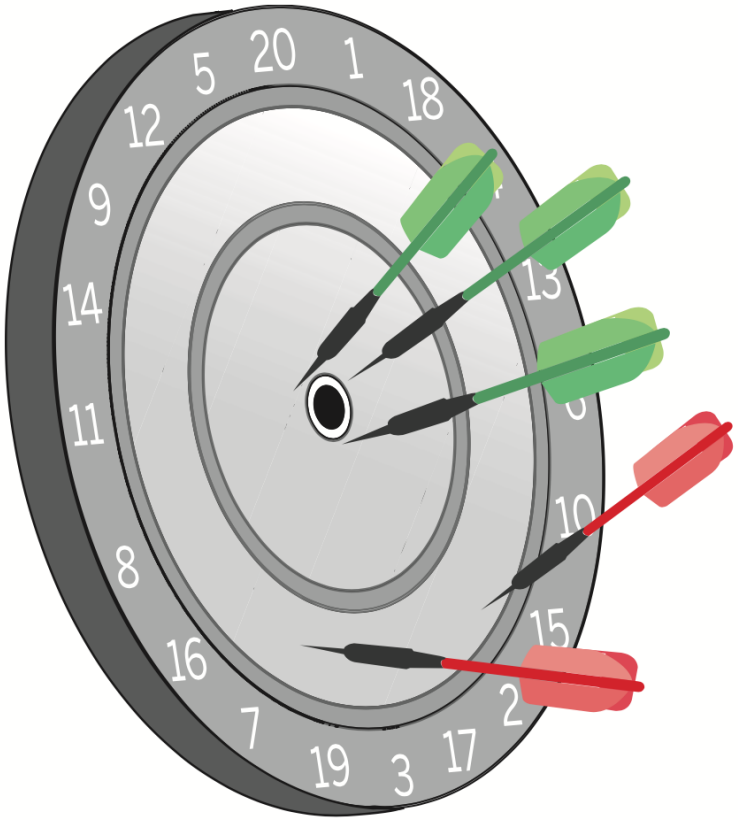
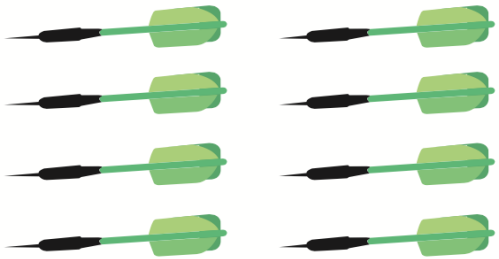
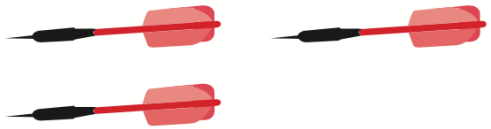
Past: Local Optimisation



New methods
Mutual agreement



Old methods
Different values



"Reproducibility in density functional theory calculations of solids"
Science 351, 1415 (2016)

Present: Global Optimisation

INPUT	OUTPUT
Composition	Structure

Imperial College London

Present: Global Optimisation

Solid State Ionics 8 (1983) 179–186
North-Holland Publishing Company

PREDICTION OF MINERAL CRYSTAL STRUCTURES

S.C. PARKER
Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK

Received 7 November 1982

The aim of our work has been to develop a computer simulation technique that can predict the structure of minerals. The basis of the technique is energy minimisation, i.e. all structural parameters are varied until the configuration with the lowest lattice energy is achieved; the initial configuration usually corresponds to an "ideal" structure based on regular polyhedra. The lattice energy is calculated using a specified potential model which includes electrostatic and short-range terms. These techniques can be applied to two distinct areas of structure prediction. The first concerns discrimination between alternative space groups proposed for the same structure. The second concerns the calculation of distortions from ideal close-packed structures. Here we concentrated mainly on silicate minerals. Furthermore, by varying the cell parameters we were able to simulate the effect of pressure on the crystal structure. Our results show that it is possible to establish potential models which predict detailed features of mineral structural chemistry.

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Present: Global Optimisation

NATURE VOL. 335 15 SEPTEMBER 1988

Crystals from first principles

A new calculation of the polymorphs of silica appears to have broken new ground in deriving crystal structure from chemical composition. But X-ray crystallographers need not worry — yet.

ONE of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition. Who, for example, would guess that graphite, not diamond, is the thermodynamically stable allotrope of carbon at ordinary temperature and pressure? Solids such as crystalline water (ice) are still thought to lie beyond mortals' ken.

oxygen atoms — the authors estimate 0.7 of an electron charge for every SiO bond, or close on two electron charges for those O atoms bound to two Si atoms. So, to ensure that their calculated structures are electrically neutral, the authors place electronic charges at points 1.65 Å along the four tetrahedral axes of the cluster, neatly simulating in the process the electrostatic effects of the neighbouring oxygen ions found in structures such as

modulus within 10 per cent. The agreement between calculated energy (enthalpy) of the polymorphs and the few measurements available is even better (1 per cent), but the authors say they could probably do even better if they allowed for the band structure of these polymorphs and the extent to which the bands are filled at different temperatures.

Several refinements remain to be explored. The chances are that three-body

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Present: Global Optimisation

Vol 457|12 February 2009|doi:10.1038/nature07736 nature

LETTERS

Ionic high-pressure form of elemental boron

Artem R. Oganov[1,2]†, Jiuhua Chen[3,4], Carlo Gatti[5], Yanzhang Ma[6], Yanming Ma[1,7], Colin W. Glass[1], Zhenxian Liu[8], Tony Yu[3], Oleksandr O. Kurakevych[9] & Vladimir L. Solozhenko[9]

Boron is an element of fascinating chemical complexity. Controversies have shrouded this element since its discovery was announced in 1808: the new 'element' turned out to be a compound containing less than 60–70% of boron, and it was not until 1909 that 99% pure boron was obtained[1]. And although we now know of at least 16 polymorphs[2], the stable phase of boron is not yet experimentally established even at ambient conditions[3]. Boron's complexities arise from frustration: situated between metals and insulators in the periodic table, boron has only three valence electrons, which would favour metallicity, but they are sufficiently

the room-temperature compression of β-B_{106} showed metastable amorphization[11] at 100 GPa and the onset of superconductivity[13] at 160 GPa. When using laser heating to overcome kinetic barriers, it was found that β-B_{106} transforms into the T-192 phase above 10 GPa at 2,280 K (ref. 14).

To further explore the intriguing high-pressure behaviour of boron, we have used 99.9999% pure β-B_{106} to synthesize (both from the melt and from the solid state) about a dozen samples containing dark-grey grains of a hitherto unknown phase of boron (see Methods for details). Single-phase samples were obtained at 12 GPa, 15 GPa

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Present: Global Optimisation

CrossMark

feature articles

Acta Cryst B
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

ISSN 2052-5206

Report on the sixth blind test of organic crystal structure prediction methods

Anthony M. Reilly,[a]* Richard I. Cooper,[b] Claire S. Adjiman,[c] Saswata Bhattacharya,[d] A. Daniel Boese,[e] Jan Gerit Brandenburg,[f]‡ Peter J. Bygrave,[g] Rita Bylsma,[h] Josh E. Campbell,[g] Roberto Car,[i] David H. Case,[g] Renu Chadha,[j] Jason C. Cole,[a] Katherine Cosburn,[k,l] Herma M. Cuppen,[h] Farren Curtis,[k,m] Graeme M. Day,[g] Robert A. DiStasio Jr,[i,n] Alexander Dzyabchenko,[o] Bouke P. van Eijck,[p]§ Dennis M. Elking,[q] Joost A. van den Ende,[h] Julio C. Facelli,[r,s] Marta B. Ferraro,[t] Laszlo Fusti-Molnar,[q] Christina-Anna Gatsiou,[c] Thomas S. Gee,[g] René de Gelder,[h] Luca M. Ghiringhelli,[d] Hitoshi Goto,[u,v] Stefan Grimme,[f] Rui Guo,[w] Detlef W. M. Hofmann,[x,y] Johannes Hoja,[d] Rebecca K. Hylton,[w] Luca Iuzzolino,[w] Wojciech Jankiewicz,[z] Daniël T. de Jong,[h] John Kendrick,[aa] Niek J. J. de Klerk,[h] Hsin-Yu Ko,[i] Liudmila N. Kuleshova,[y] Xiayue Li,[k,bb] Sanjaya Lohani,[k] Frank J. J. Leusen,[aa] Albert M. Lund,[q,cc] Jian Lv,[dd] Yanming Ma,[dd] Noa Marom,[k,ee] Artëm E. Masunov,[ff,gg,hh,ii] Patrick McCabe,[a] David P. McMahon,[g] Hugo Meekes,[h] Michael P. Metz,[jj] Alston J. Misquitta,[kk] Sharmarke Mohamed,[ll] Bartomeu Monserrat,[mm,nn] Richard J. Needs,[mm] Marcus A. Neumann,[oo] Jonas Nyman,[g]

Received 15 February 2016
Accepted 4 May 2016

Edited by C. H. Görbitz, University of Oslo, Norway

‡ Present Address: Department of Chemistry, London Centre for Nanotechnology, University College London, 20 Gordon Street, London WC1H 0AJ, England.
§ Retired.

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Future: Materials Design

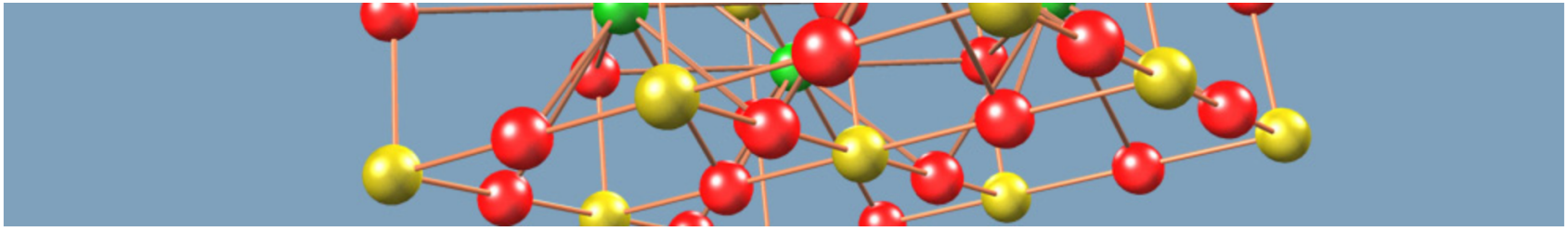
INPUT	OUTPUT
Property	Composition Structure

Imperial College London

Future: Materials Design (USA)

Center for Inverse Design

Achieving the grand challenge of materials and nanostructures by design



- About the Center
- Approach
- Publications

Center for Inverse Design

The Center for Inverse Design (CID) was a first-generation (2009–2014) Energy Frontier Research Center funded by the U.S. Department of Energy Office of Science. To address a crucial scientific grand challenge, the Center developed and utilized a new approach to material science. As shown in the figure below, rather than using the conventional direct approach ("Given the structure, find the electronic properties"), we used a "materials by inverse design" approach ("Given the desired property, find the structure").

Comparison of the "materials by inverse design" approach (left to right) versus the conventional approach (right to left)

The target properties of interest include general semiconductor optical and electrical properties; the desired materials functionalities include electron- and hole-conductive

Quick Links

- **Reinventing Material Science** (Continuum Magazine, 10/2012)
- **The Mystery of the Missing Materials**
- **Inverse Design summer school brochure, 9/2011**
- **Center for Inverse Design poster for EFRC Summmit, 5/2011**
- **Center for Inverse Design fact sheet**
- **Energy Frontier Research Center slide**
- **NREL gets $20M from DOE for solar** (Denver Business Journal, 8/6/09)
- **NREL Center Turns Materials Design Upside Down** (NREL news feature, 8/14/09)

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Future: Materials Design (UK)

MATERIALS INNOVATION FACTORY

Computer Aided Material Science

Computer aided modelling has revolutionised many aspects of modern life from architecture to product design.

Its impact on chemistry has to date been limited.

Through the use of Computer Aided Materials Science (CAMS) and high-throughput (HT) automation, the Materials Innovation Factory aims to address this

The potential that new forms of computing and automation can bring to research is near limitless.

Imperial College London

Future: Materials Design (UK)

OVERVIEW OUR THEMES MEMBERS PUBLICATIONS EVENTS OUTPUTS CONTACT

MEMBERS

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Cardiff University
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University of Bath
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University of Bath
website • email

Prof Aron Walsh
Imperial College London
website • email

Dr Ilian Todorov
STFC - Laboratories
website • email

Imperial College London

Future: Materials Design (EU)

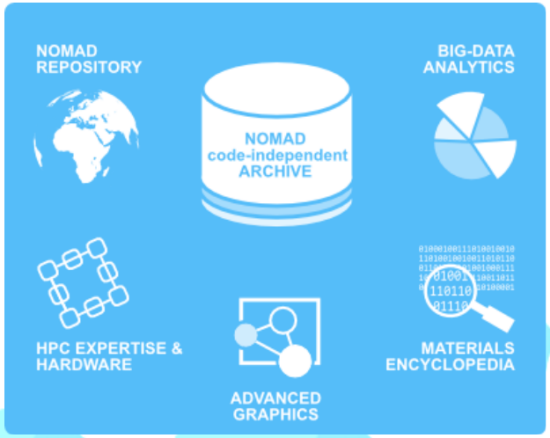
NOMAD

THE NOMAD LABORATORY
A EUROPEAN CENTRE OF EXCELLENCE

HOME PROJECT INDUSTRY OUTREACH TEAM CODES NEWS PRESS KIT CONTACT US

Enter Search...

The Novel Materials Discovery (NOMAD) Laboratory develops a *Materials Encyclopedia* and *Big-Data Analytics* and *Advanced Graphics Tools* for materials science and engineering.



NOMAD
STRUCTURE AND USE CASES

Latest News

Feb 23, 2017
NOMAD Video of Carbon Dioxide interacting with a CaO surface

Feb 22, 2017
NOMAD Computer scientist position at the Fritz Haber Institute, Berlin

Feb 22, 2017
New publication from HUB

Feb 20, 2017
Berlin Big Data Research Newsletter

Imperial College London

Computational Property Databases

- http://aflowlib.org
- https://materialsproject.org
- http://repository.nomad-coe.eu
- http://materials.nrel.gov
- http://oqmd.org
- http://phonondb.mtl.kyoto-u.ac.jp
- http://www.tedesignlab.org

"We now need a database of databases"

Jonathan Skelton (University of Bath), 2015

Imperial College London

Materials Project

The Materials Project

Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

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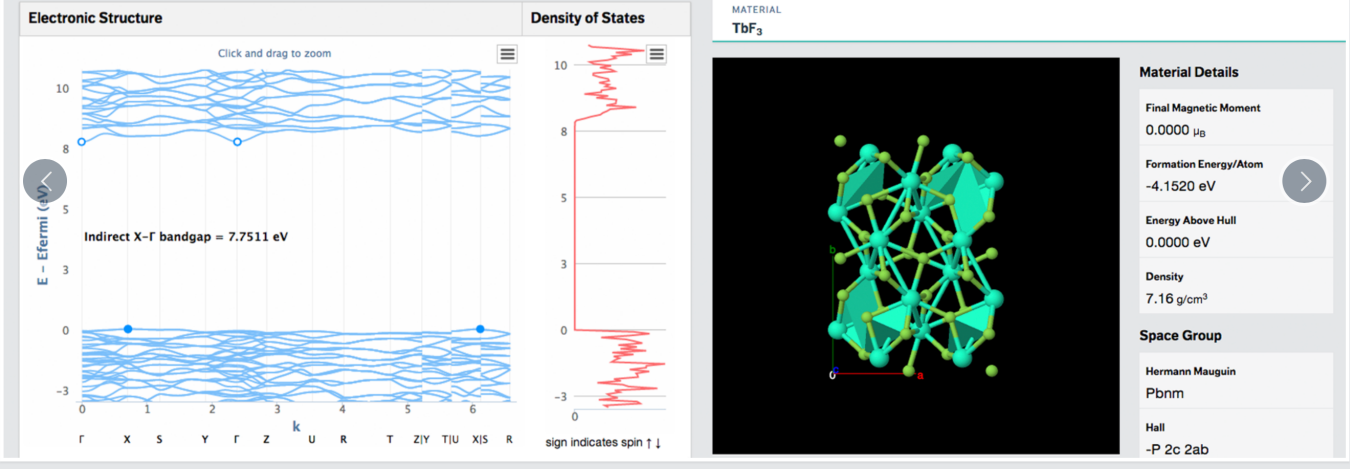

EXPLORE MATERIALS
Search for materials information by chemistry, composition, or property

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

VISUALIZE STABILITY
Generate phase and pourbaix diagrams to find stable phases and study reaction pathways

INVENT STRUCTURES
Design new compounds with our structure editor and substitution algorithms

CALCULATE
Calculate the enthalpy of 10,000+ reactions and compare with experimental values

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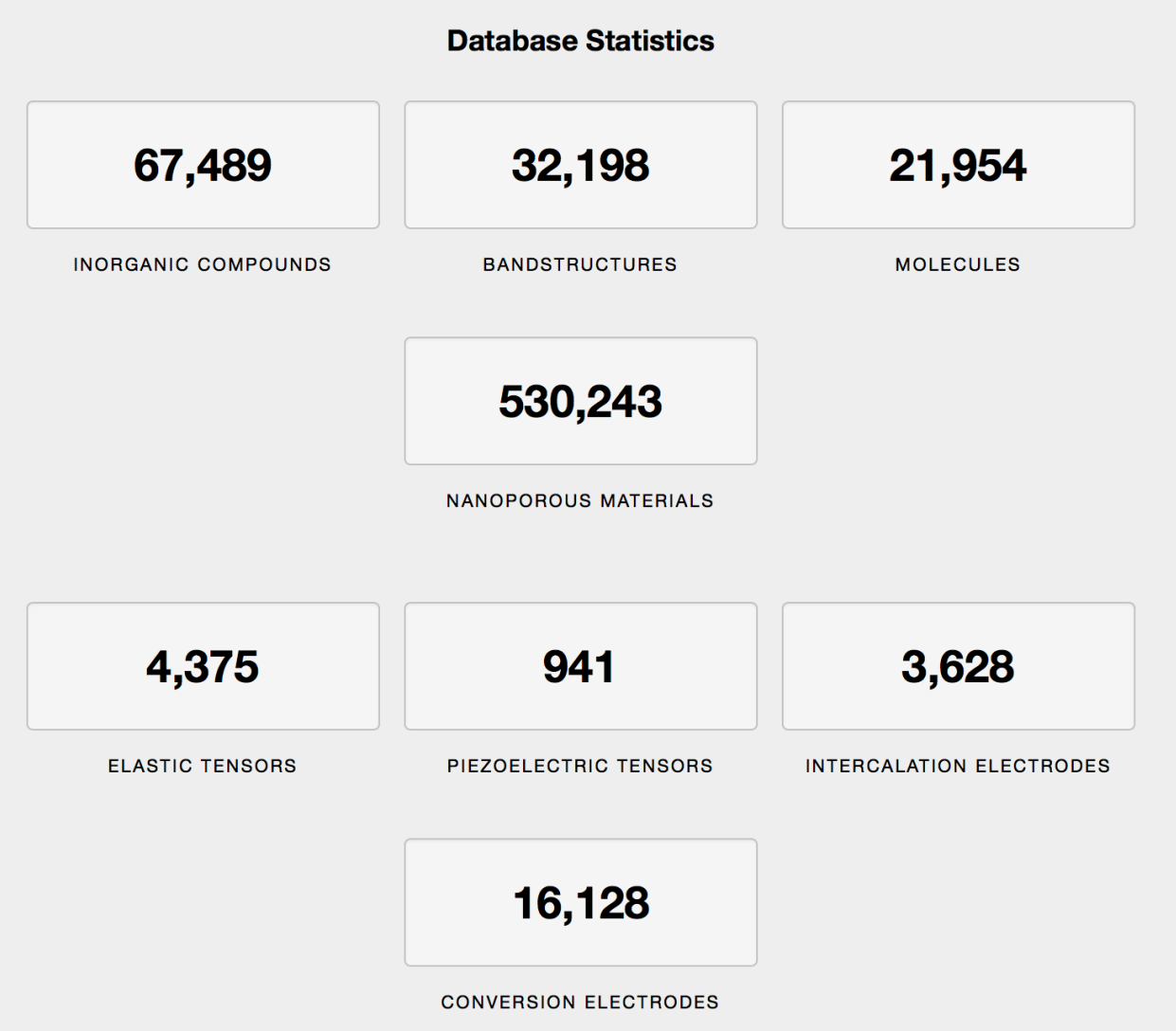
Materials Project



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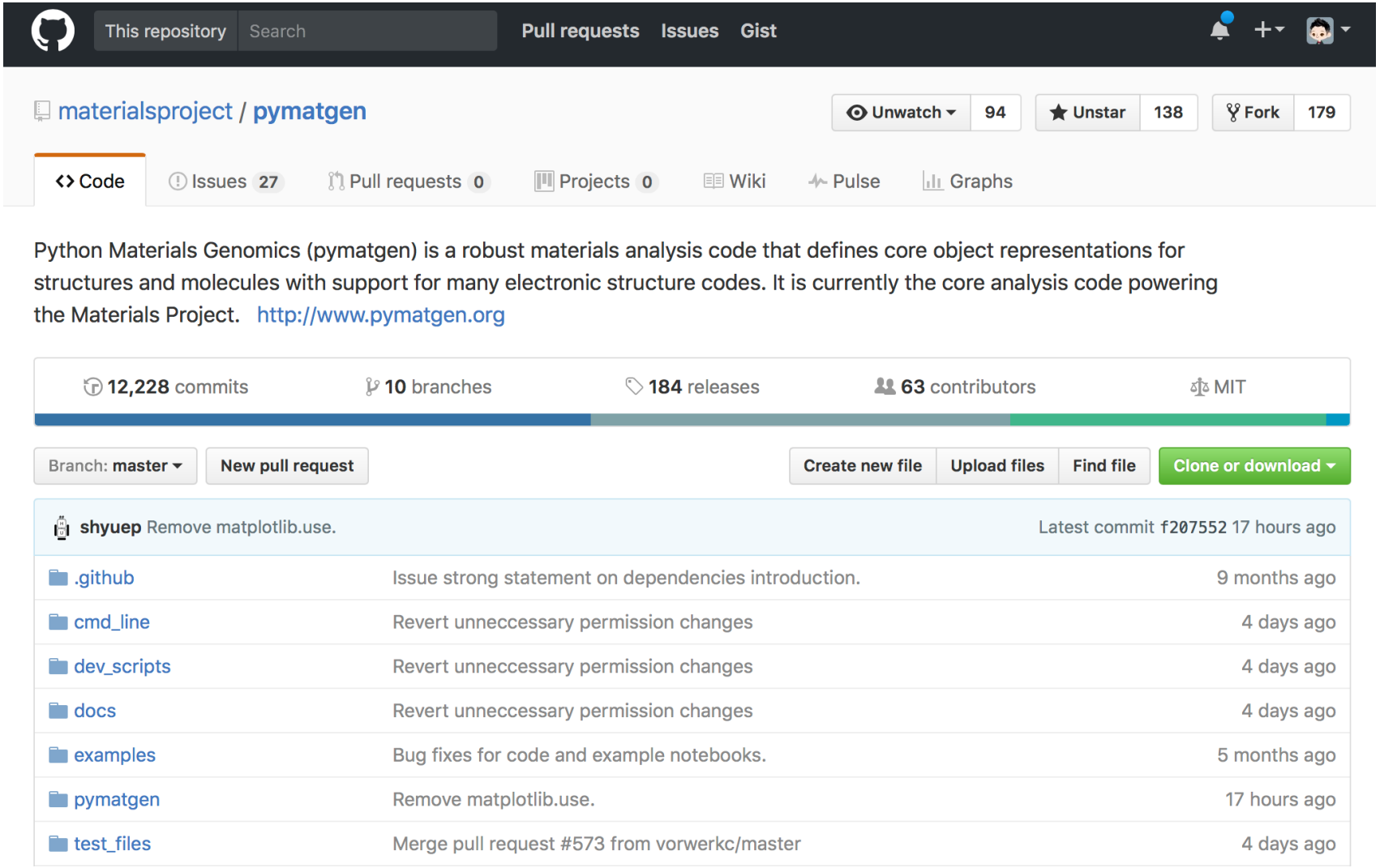
Materials Project (Open Source)



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Talk Outline

1. Materials Modelling in 2017
2. From Atoms to Devices

Imperial College
London

Games Are Fun (And Useful)

Imperial College London

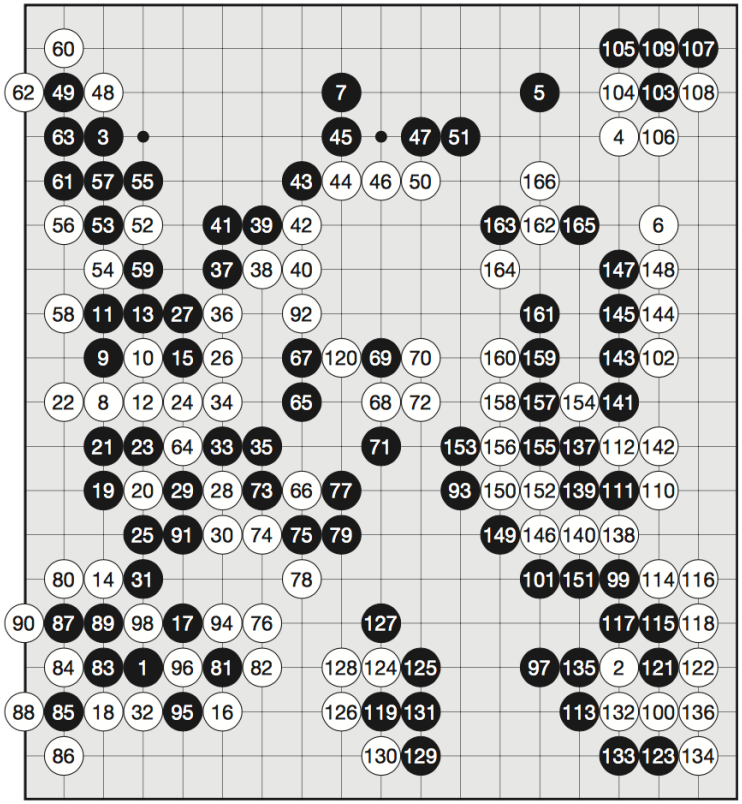
Confucius (China, 500 BCE)

Gentlemen should not waste their time on trivial games – they should study go.

Imperial College London

Combinatorial Explosion

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



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

~ 10^{80} atoms in the universe

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Alpha Go

ARTICLE

doi:10.1038/nature16961

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

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

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

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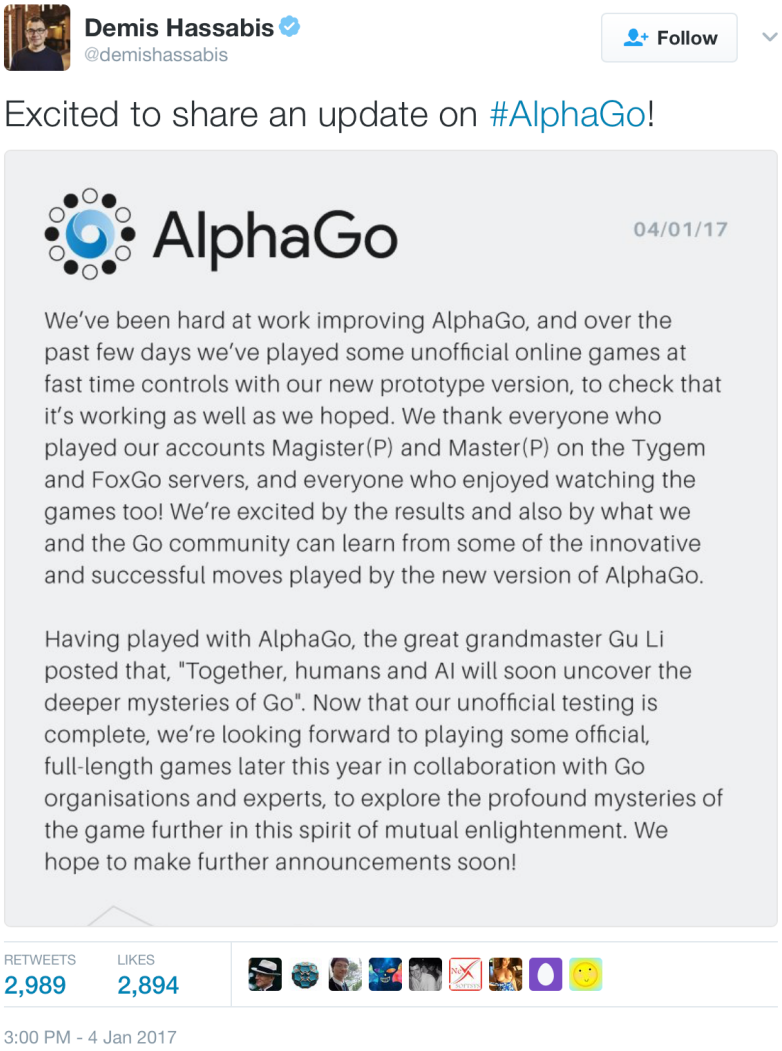
Alpha Go Master (Superhuman)



Late 2016:

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

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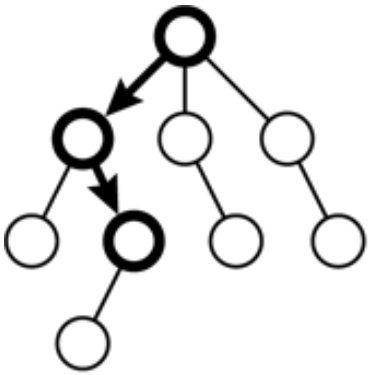
Inside Alpha-Go

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

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

- $10 \times 10 \times 10$ lattice
- 50 elements
- $50^{1000} = 10^{1968}$

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Materials Hyperspace

Type and ratio of ions with their arrangement in space

How to find the optimal materials for:

Property / Performance / Sustainability

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Computational Materials Design

INPUT	OUTPUT
Property	Composition Structure

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

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Computational Materials Design

INPUT	OUTPUT
Property	Composition Structure

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

} "Materials Genome"

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Predicting Functional Materials (1964)

J. Phys. Chem. Solids Pergamon Press 1964. Vol. 25, pp. 675–684. Printed in Great Britain.

A SYSTEMATIC METHOD OF DERIVING NEW SEMICONDUCTING COMPOUNDS BY STRUCTURAL ANALOGY

B. R. PAMPLIN

Physics Department, Bristol College of Science and Technology

(*Received* 21 *October* 1963; *in revised form* 27 *January* 1964)

Abstract—A method of deriving new semiconducting compounds and alloys is described using mathematical formulae derived by considering the rules of valency and structural analogy. The method is applied to tetrahedral inorganic compounds and used to tabulate known tetrahedral phases and predict a large range of probable new ones. All these phases if formed will be semiconducting. Ternary and quaternary compounds and alloys are discussed in detail and more complex ones mentioned.

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Machine Learning (1998)

Journal of ALLOYS AND COMPOUNDS

Journal of Alloys and Compounds 279 (1998) 8–13

Computational materials design using artificial intelligence methods

N.N. Kiselyova[a,*], V.P. Gladun[b], N.D. Vashchenko[b]

[a]*A.A. Baikov Institute of Metallurgy, Russian Academy of Sciences, Leninskii Prospect, 49, 117334 Moscow, Russia*
[b]*Institute of Cybernetics, National Academy of Sciences of Ukraine, Prospect Acad. Glushkova, 40, 252650, GSP, Kiev-22, Ukraine*

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London

Data Mining (2003)

Journal of
MOLECULAR
STRUCTURE

Journal of Molecular Structure 647 (2003) 17–39

www.elsevier.com/locate/molstruc

Crystal structure prediction by data mining

Detlef W.M. Hofmann[a,*], Joannis Apostolakis[b]

[a]*Department of Inorganic chemistry, University Frankfurt, Marie-Curie-str.11,60439 Frankfurt, Germany*
[b]*Fraunhofer Institute for Algorithms and Scientific Computing, Schloss Birlinghoven, D-53754 Berlin, Germany*

Received 10 November 2001; revised 5 March 2002; accepted 5 March 2002

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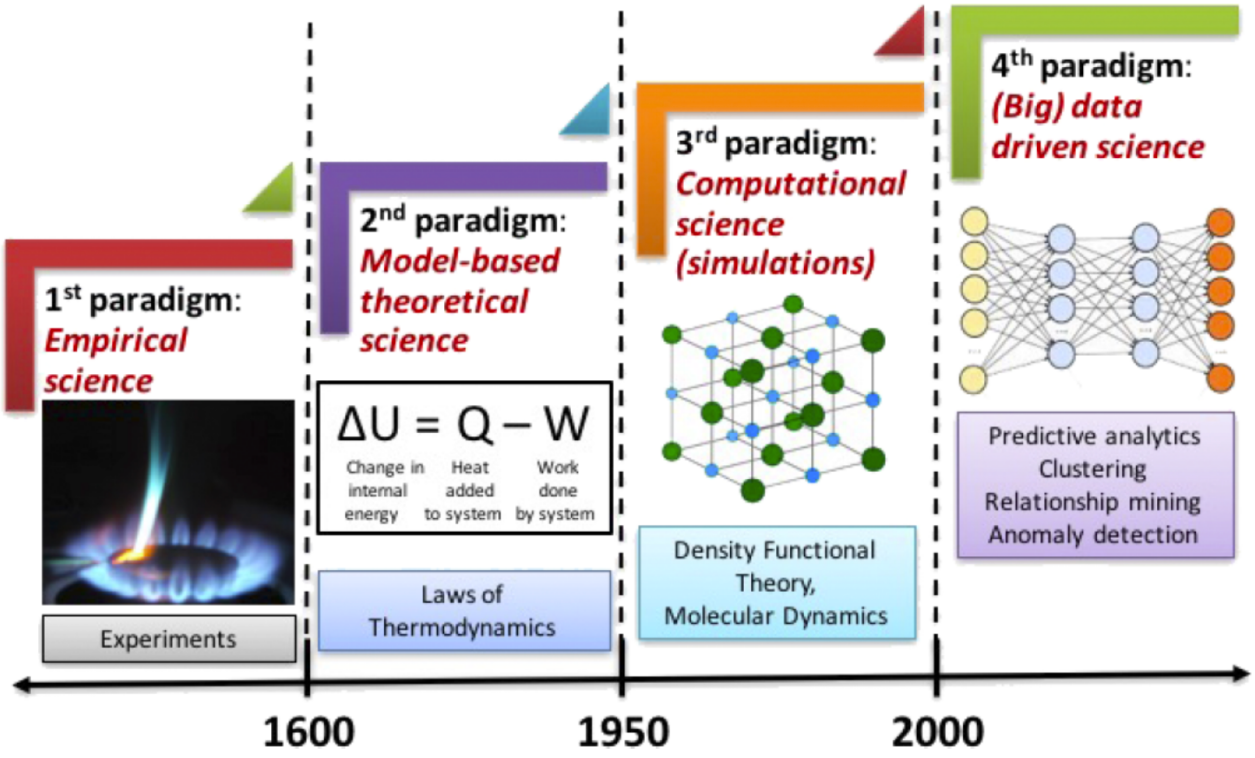
New Paradigm in Science

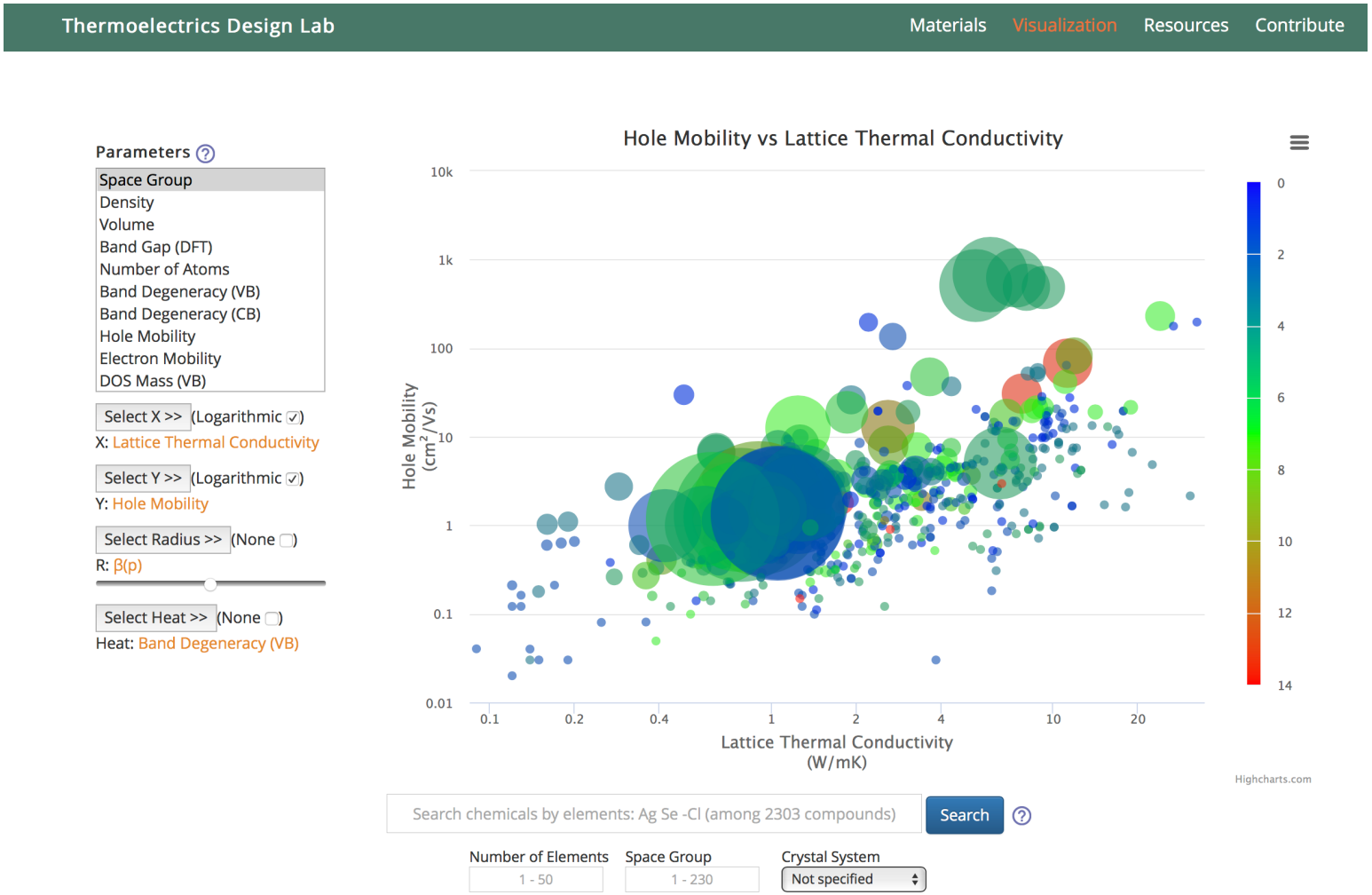
Global Movement Associated with Databases, #OpenData and #OpenScience



Agrawal and Choudhary, APL Materials 4, 053208 (2016)

Imperial College London

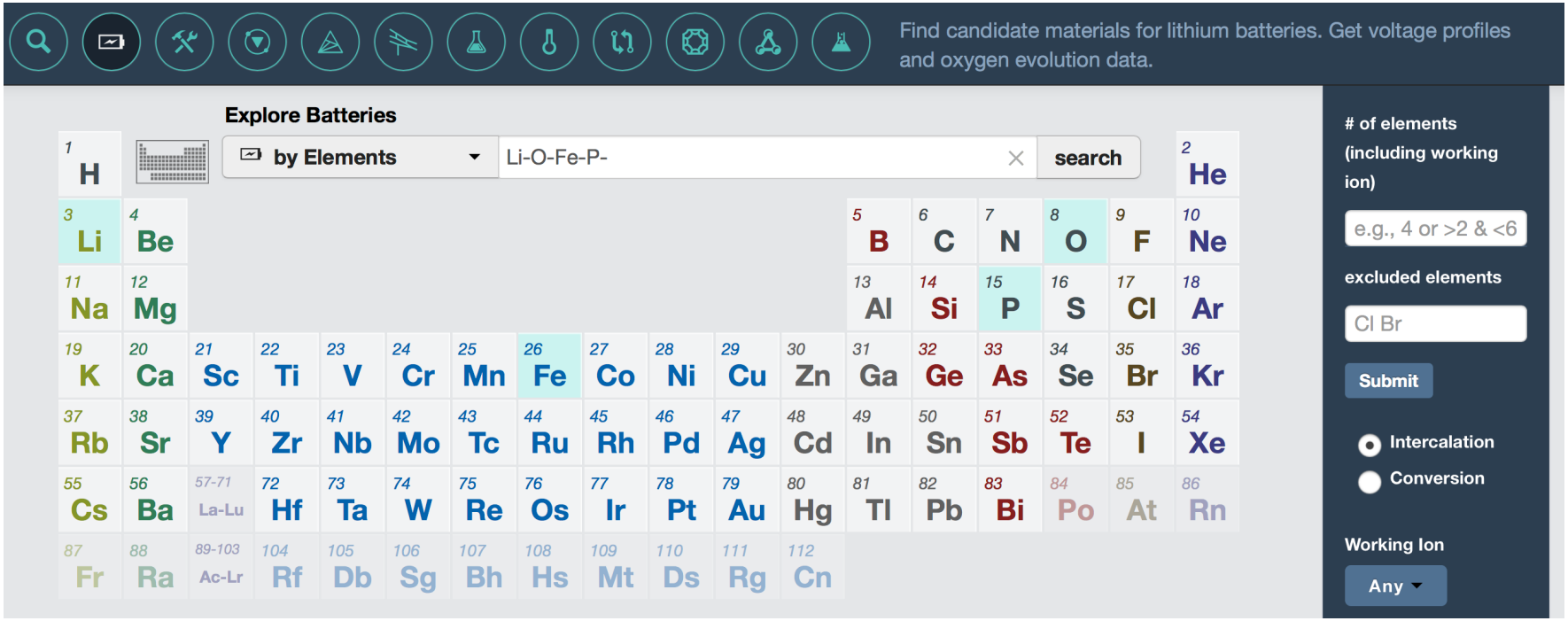
Thermoelectrics: Heat to Electricity



http://www.tedesignlab.org

Imperial College London

Batteries: Electrical Energy Storage



https://materialsproject.org

Imperial College London

Photovoltaics: Light to Electricity

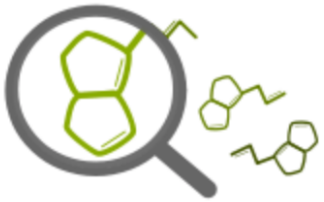
molecular space

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.

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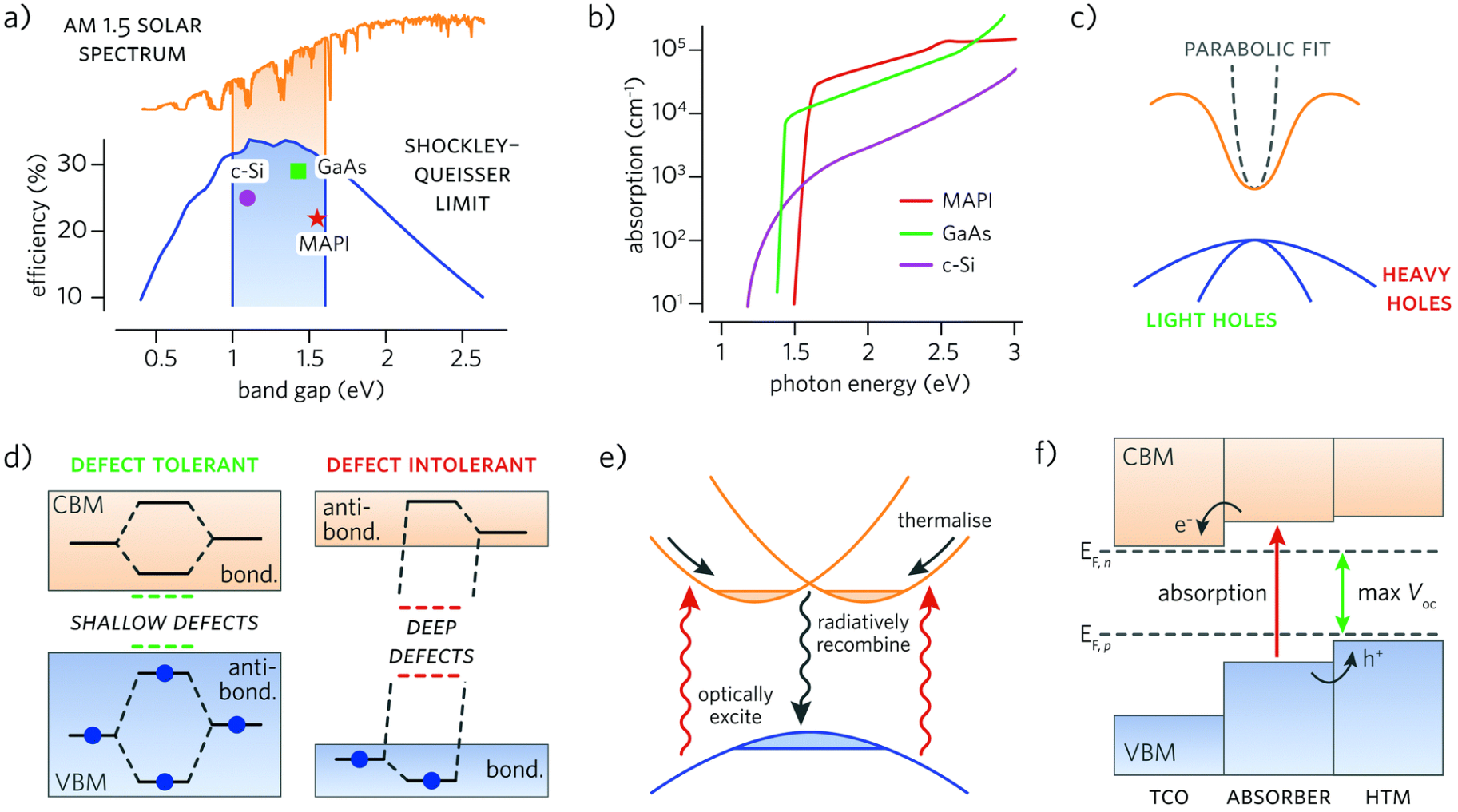
Photovoltaics: Light to Electricity



A. M. Ganose et al, Chem. Comm. 53, 20 (2017)

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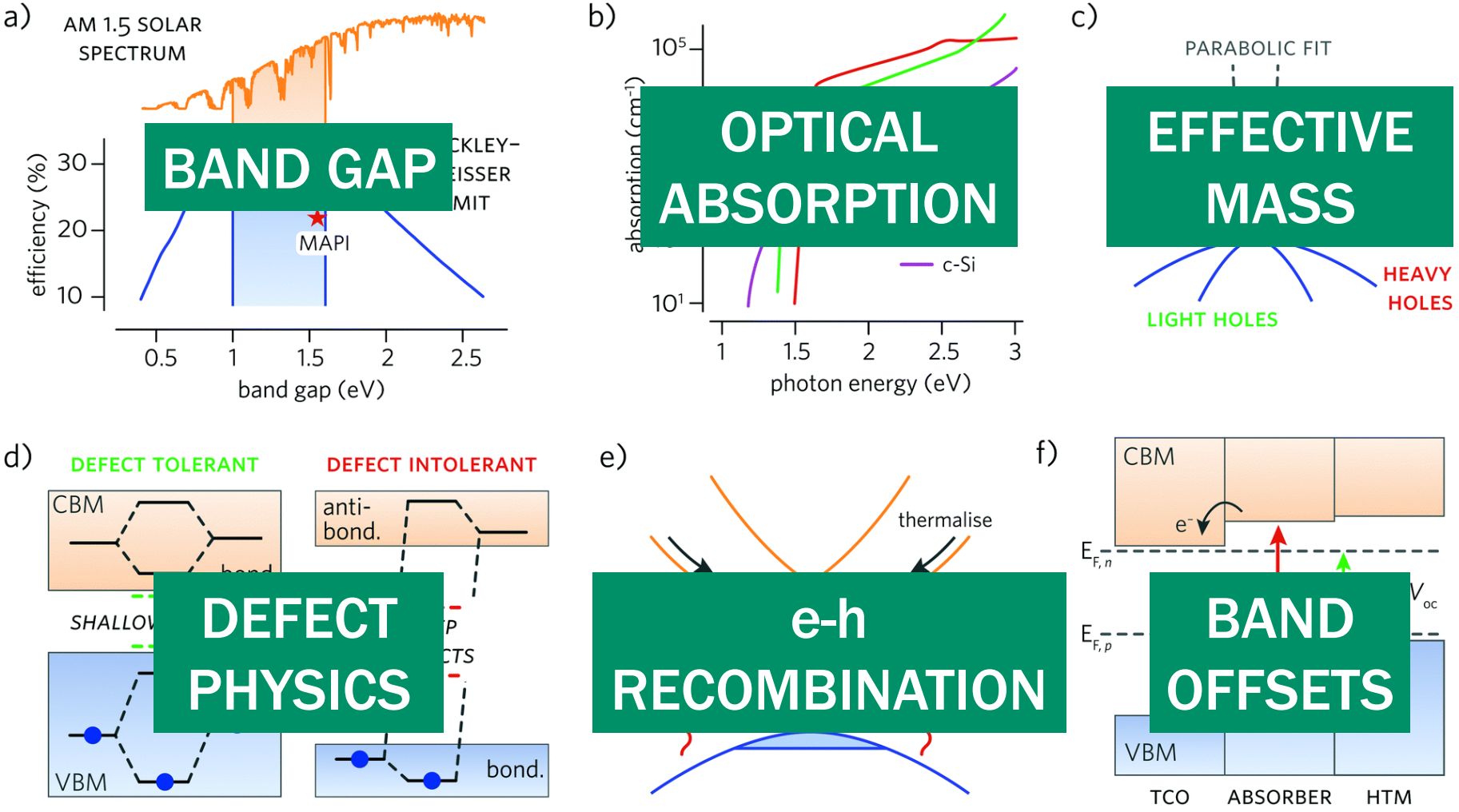
Photovoltaics: Light to Electricity



A. M. Ganose et al, Chem. Comm. 53, 20 (2017)

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Infrastructure for 10^{100} Materials

Chem

CellPress

Article

Computational Screening of All Stoichiometric Inorganic Materials

Daniel W. Davies,[1,4] Keith T. Butler,[1,4] Adam J. Jackson,[1,4] Andrew Morris,[1] Jarvist M. Frost,[1] Jonathan M. Skelton,[1] and Aron Walsh[1,2,3,5,*]

Open Source Python Package

https://github.com/WMD-group/SMACT

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Infrastructure for 10^{100} Materials

Compositional Combinations

Chemical Filters

Structure Prediction

[LO-FI]

[HI-FI]

Structure Prediction

Property Calculation

Final Candidates

Imperial College London

From Materials to Devices

Computational procedure for assessing and screening materials interfaces

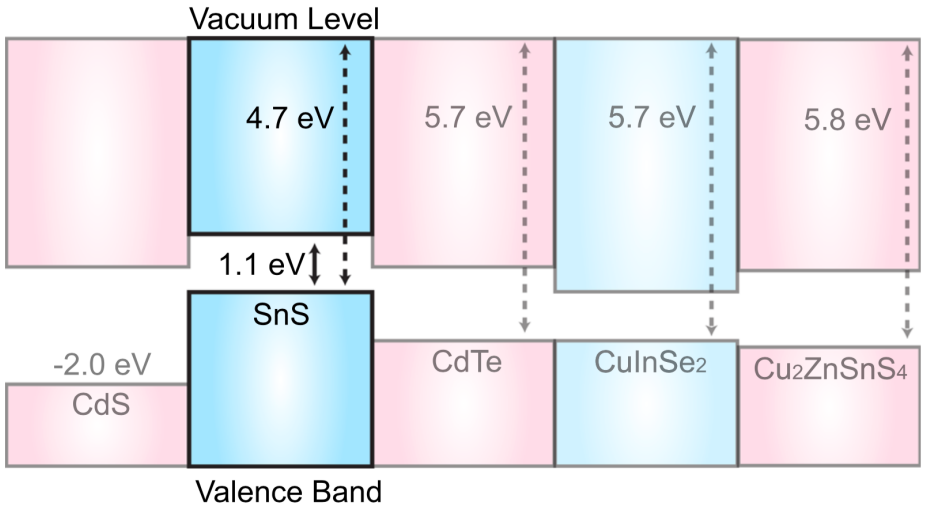
Lattice strain / Site overlap / Electronic matching

Lattice match: An application to heteroepitaxy

A. Zur and T. C. McGill
California Institute of Technology, Pasadena, California 91125

(Received 11 July 1983; accepted for publication 20 September 1983)

We define the concept of lattice match for any pair of crystal lattices in any given crystal direction, allowing for a periodic reconstruction of the interface. An algorithm for a systematic search for all possible matches is developed, and some examples of nonstandard lattice matches are given for CdTe on GaAs and sapphire to illustrate the method. For the case of CdTe on GaAs, our results agree with published results, both with respect to growth plane and orientation for CdTe(111) on GaAs(100). For CdTe on sapphire, our results agree with published results with respect to growth plane.



K. T. Butler et al, J. Mater. Chem. C 4, 1129 (2016)

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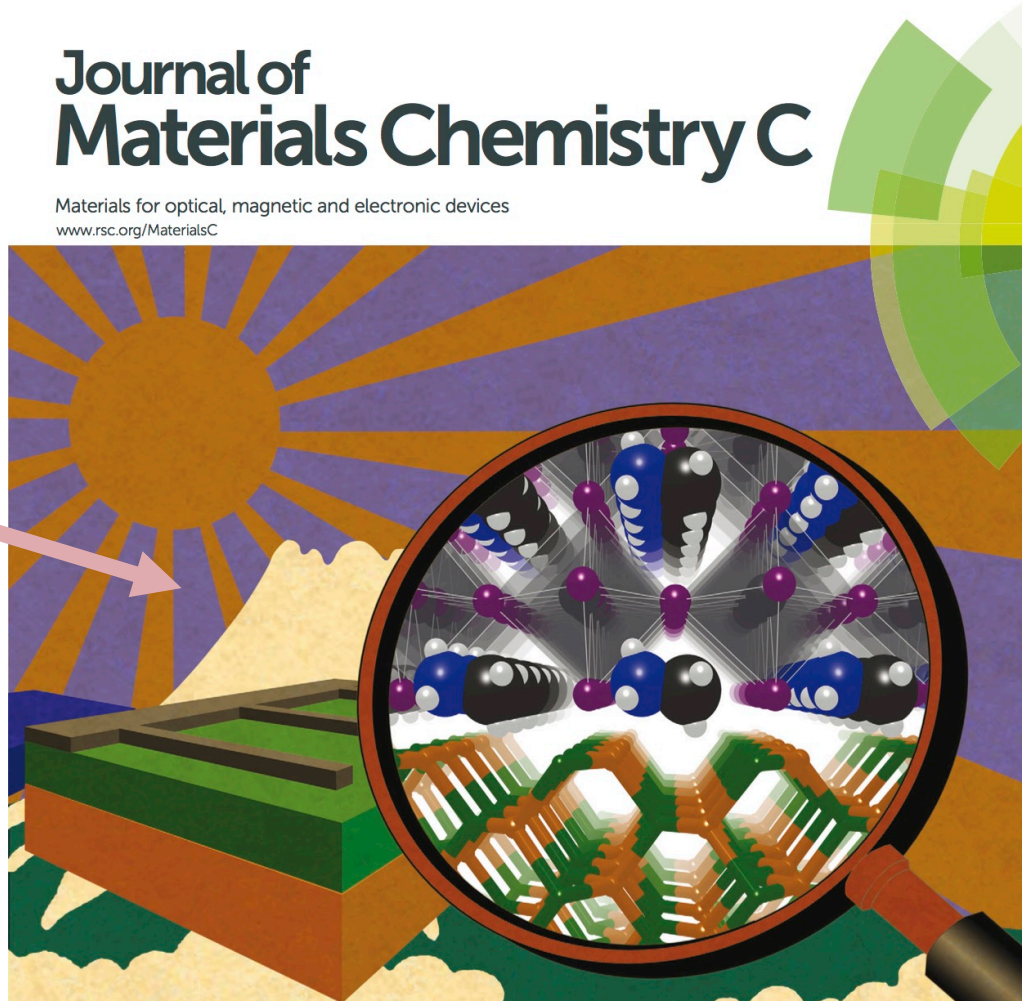
From Materials to Devices

Collaboration with Tokyo Institute of Technology supported by JSPS



K. T. Butler et al, J. Mater. Chem. C 4, 1129 (2016)

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Talk Motivation

New Materials for Energy Technologies

- Performance
- Cost
- Stability
- Sustainability

Is computational materials design now a reality? Almost...

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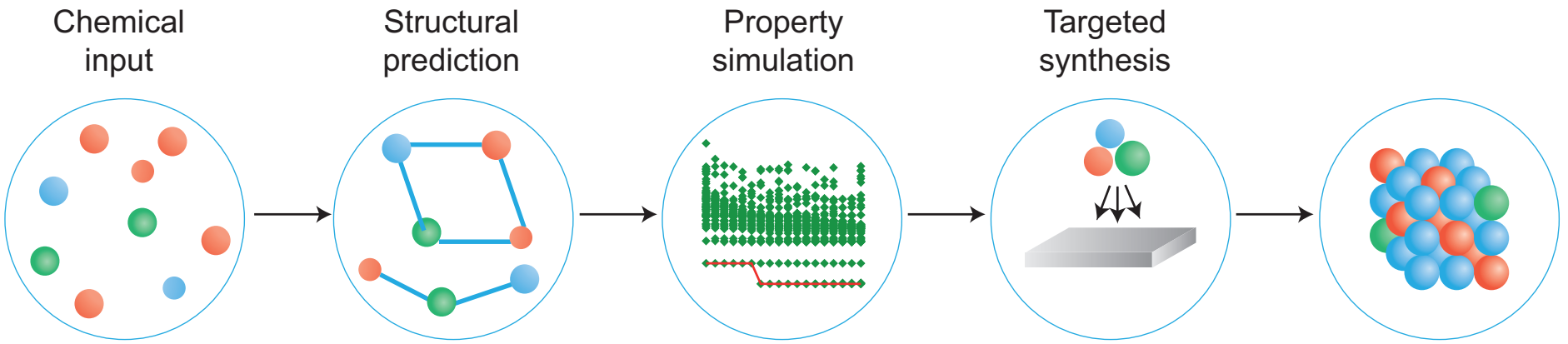
From Atoms to Devices



A. Walsh, Nature Chemistry 7, 274 (2015)

EPSRC
Engineering and Physical Sciences Research Council

The Leverhulme Trust

erc

THE ROYAL SOCIETY

European Commission

Horizon 2020
European Union funding for Research & Innovation

Slides: https://speakerdeck.com/aronwalsh