计算科学初探

Computational Science 101

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FUNSOM

Soochow University

Course Related

- Time: Mon, Class 3&4, 605-5201
- Teaching Assistant: Ms. Jie Luo
  Mr. Xiaodong Yan
  Mr. Xingxing Wen

上午11:52 | 7.7K/s

群聊二维码

计算科学初探2022...

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Syllabus

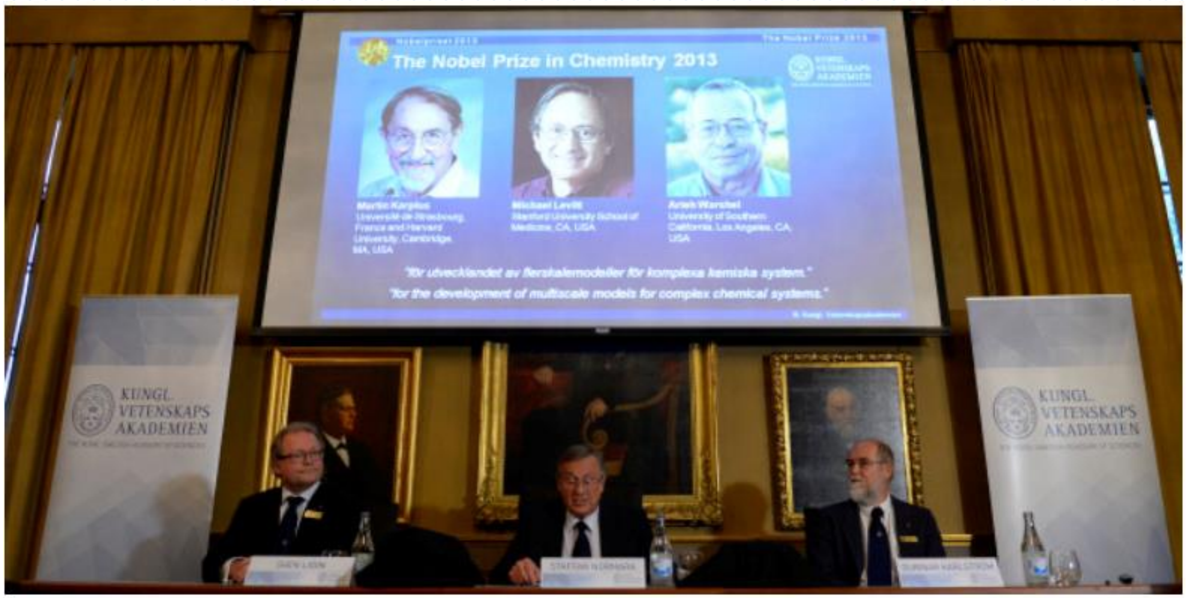
Week	Date	Topic
2	5 Sep	Introduction & Materials Genome Initiative
4	16 Sep	Big Data
5	19 Sep	Fundamentals of Machine Learning I Attendance
7	10 Oct	Fundamentals of Machine Learning II Attendance
8	17 Oct	Fundamentals of Machine Learning III
9	24 Oct	Fundamentals of Machine Learning IV Attendance
10	31 Oct	Fundamentals of Machine Learning V
11	7 Nov	Project Practice I Attendance
12	14 Nov	Project Practice II
13	21 Nov	Project Practice III Attendance
14	28 Nov	Essay Presentation I
15	5 Dec	Essay Presentation II
16	12 Dec	Essay Presentation III
17	19 Dec	Essay Presentation IV + Review

Assessments

Overall grading

Project	30%
Final Exam	50%
Attendance	5%
Presentation	15%
	100%

Introduction



Karplus Levitt Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems".*

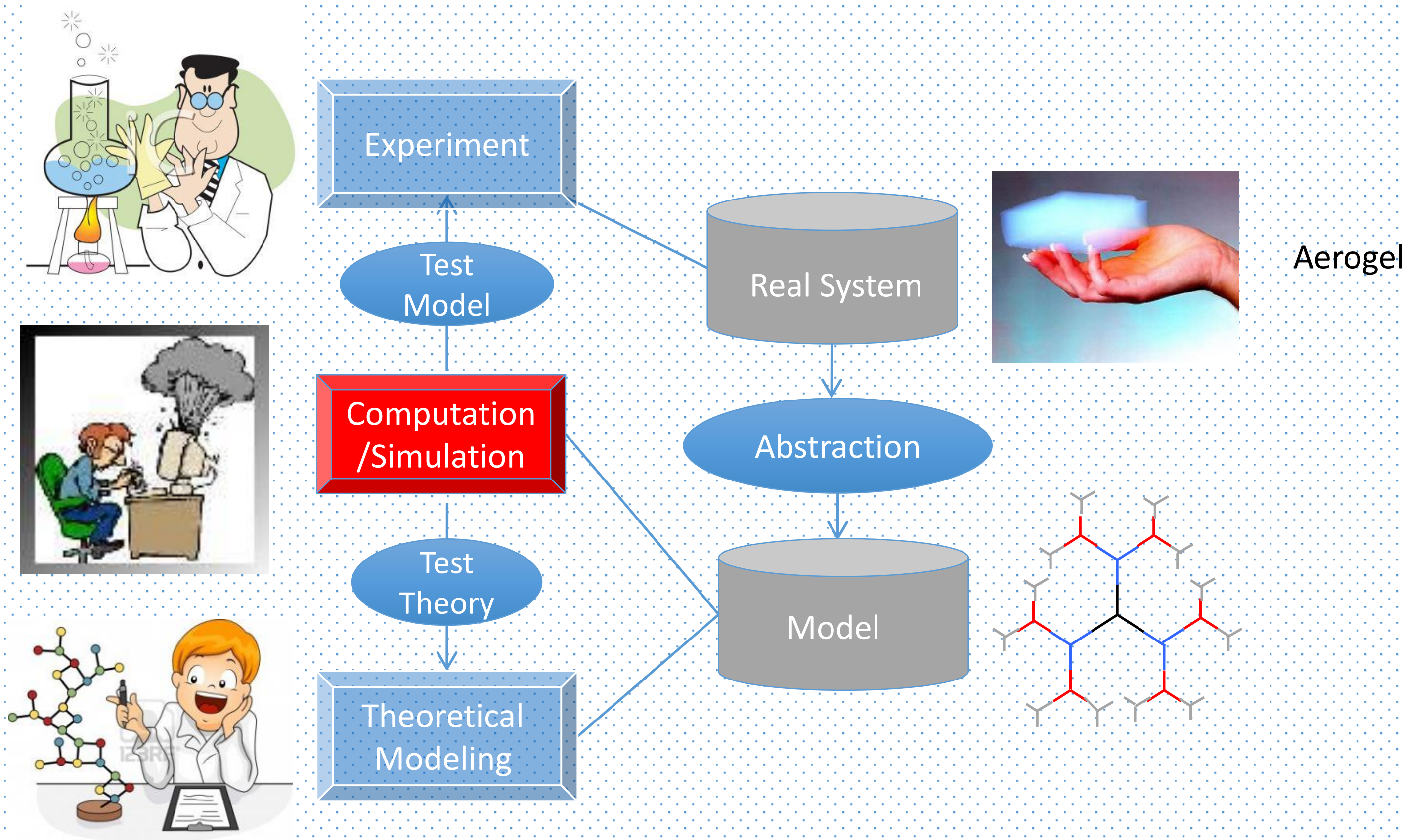
The Nobel Prize in Chemistry 2013

Multi-Scale Model

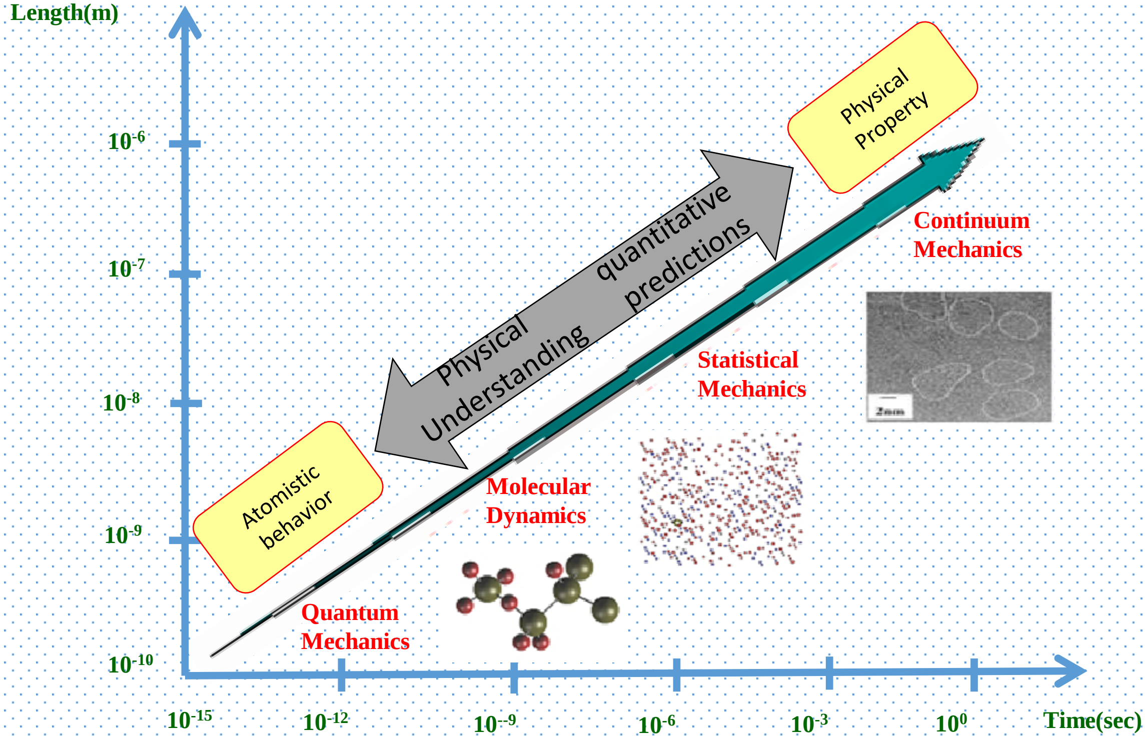
CEO of AIP: John Haynes

“Today's Nobel Prize announcement is a great example of how the study of Physics, Chemistry and Biology are crossing traditional boundaries to help tackle tough problems ranging from designing new materials for renewable energy to pharmaceutical drug design.”

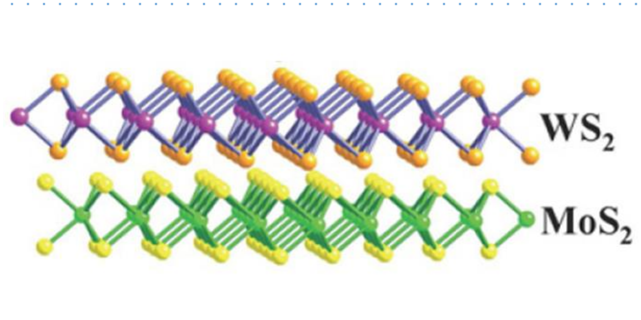
Computational Science: The Bridge

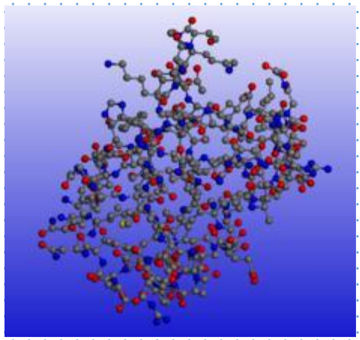


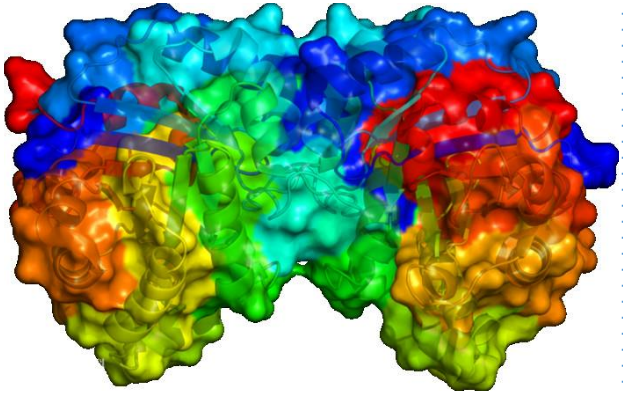
How long? How large?



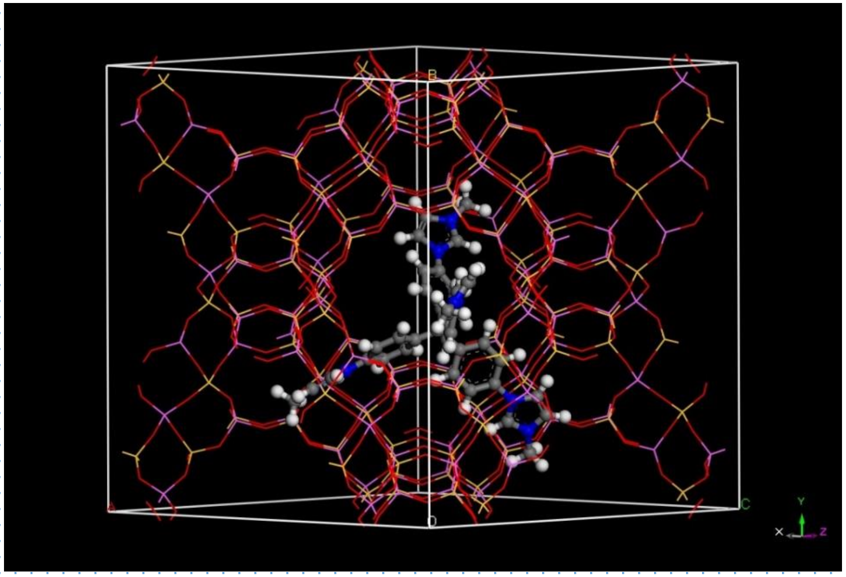
Multiscale

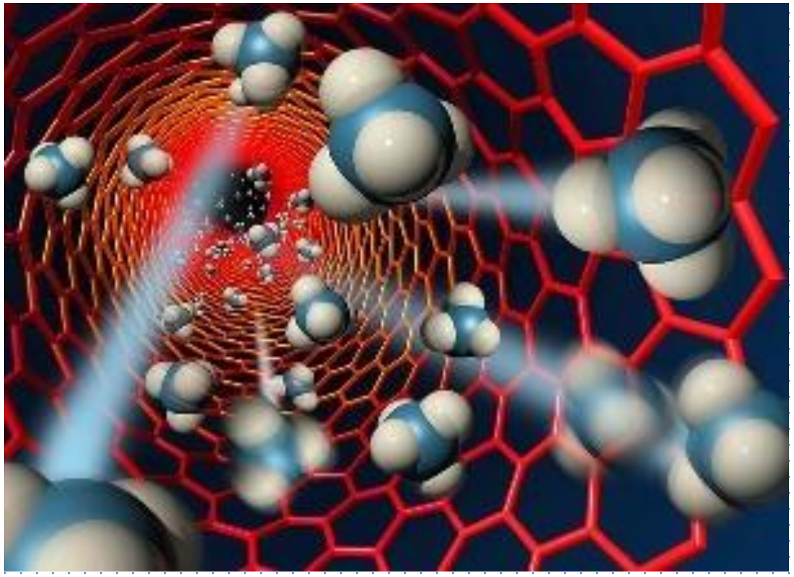






Multiscale





Role Model

D. E. Shaw
PhD@Stanford
Professor@Columbia
Parallel computing

Wall Street
Morgan Stanley
Quant trading

D.E. Shaw & Co. LP
41 billion dollar

Supercomputer

Computational Chemistry

General purpose computing

PhD@Computational Chemistry
PhD@Computational Biophysics
PhD@Electrical Engineering
IMO Medal
IPhO Medal
IChO Medal
IBO Medal

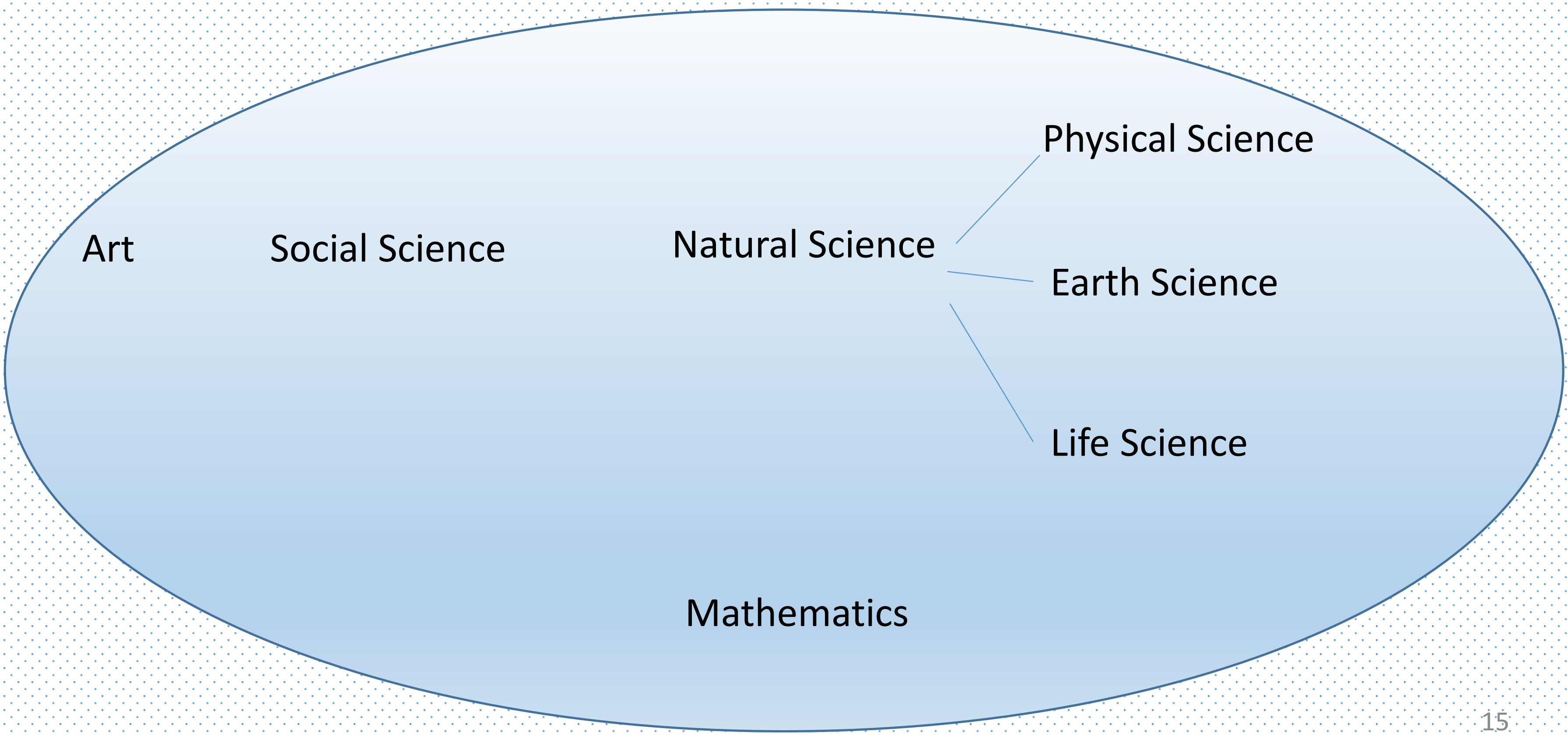
Special purpose computing
Anton

Now,

Object-Oriented &

Being a Well-rounded Individual…

Science and Art
East and West
Everything is connected…
Connecting the dots…



Materials Genome Initiative

The Announcement

Announced in June 2011 at Carnegie Mellon University:
“To help businesses discover, develop, and deploy new materials twice as fast, we’re launching what we call the **Materials Genome Initiative**. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.”

http://www.whitehouse.gov/mgi

The Objectives

Basic Goal: Reduce time-to-market for new materials for 50% or more.

- ✓ Develop a Materials Innovation Infrastructure
- ✓ Use advanced materials to reach goals in energy, security and human welfare
- ✓ Educate the next generation materials workforce

Precursors

The origin of the MGI reaches back in time…

- ✓ Academic research efforts (Steel Research Group /QuesTek (1990s)
- ✓ 2004 NRC report, uses “genome” terminology
- ✓ DARPA AIM
- ✓ ICME, successful aluminum alloy design
- ✓ Others…

Multi-agency formulation

The MGI’s origin also span many agencies…

NIST, DOE, NSF, DOD worked with OSTP to prepare the initial MGI white paper (2010-2011)

Precursor themes

These all had unifying themes:

- ✓ Bridge modeling length scales (Some institutions have these under one roof)
- ✓ Use and/or build databases
- ✓ Solve the "inverse problem" – design a material!

Sound like anyone you know?

The issues addressed, and the breadth of scope, are familiar to the Python and SciPy communities.

SciPy is about the tools.

- ✓ SciPy co-hosted with DDANSE neutron-data effort, 2006
- ✓ Focus area on data science, 2011
- ✓ Focus area on machine learning, 2013
- ✓ Focus area on reproducible science, 2013

Government-wide response

MGI is administered by an NSTC Subcommittee whose members include NIST, DOE, DOD, NSF, NASA, NIH, USGS, and OMB.

This breadth reflects the breadth of the task, which calls for efforts in data science, workflow tools, parallel and high-performance computing, and high-throughput techniques of various kinds, as well as education.

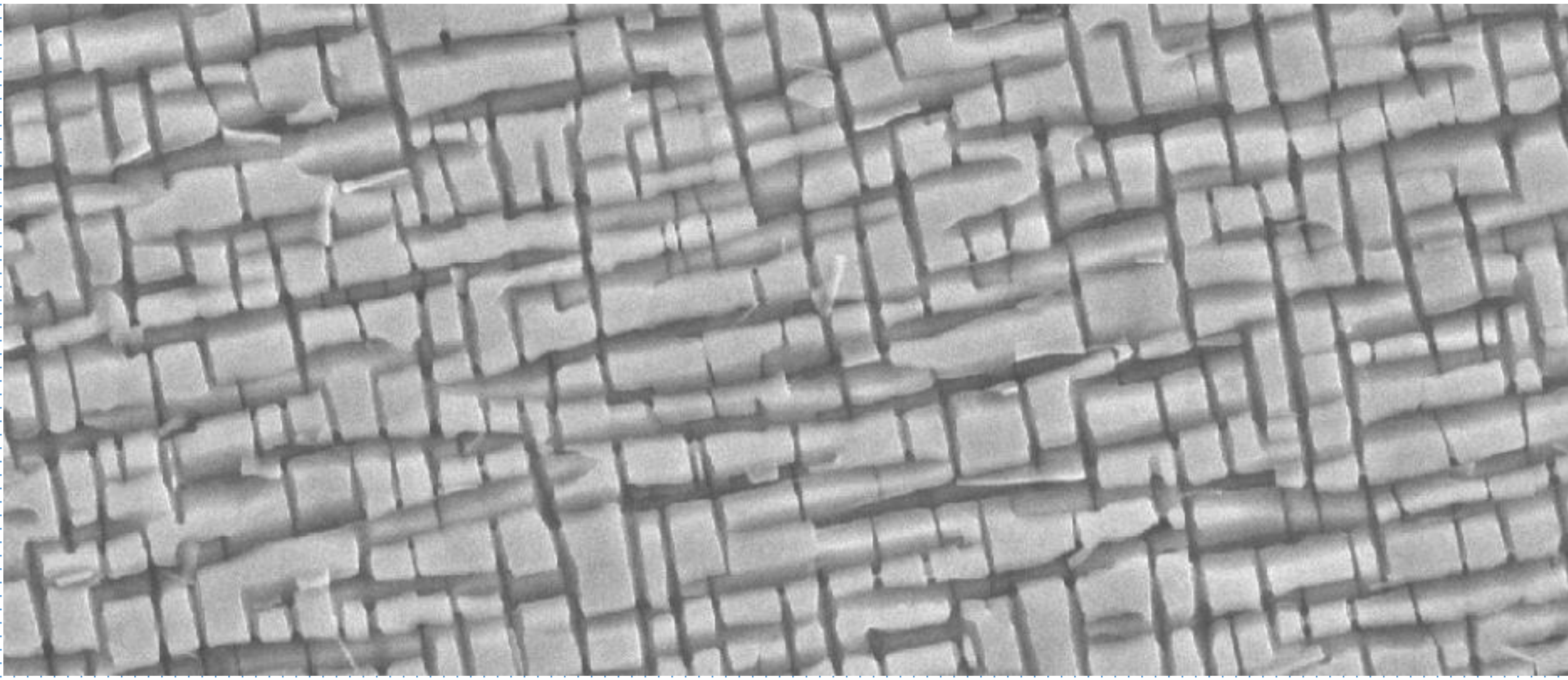
Materials Genome Initiative

Multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost.

Advanced materials are essential to economic security and human well being, with applications in industries aimed at addressing challenges in clean energy, national security, and human welfare, yet it can take 20 or more years to move a material after initial discovery to the market. Accelerating the pace of discovery and deployment of advanced material systems will therefore be crucial to achieving global competitiveness in the 21st century.

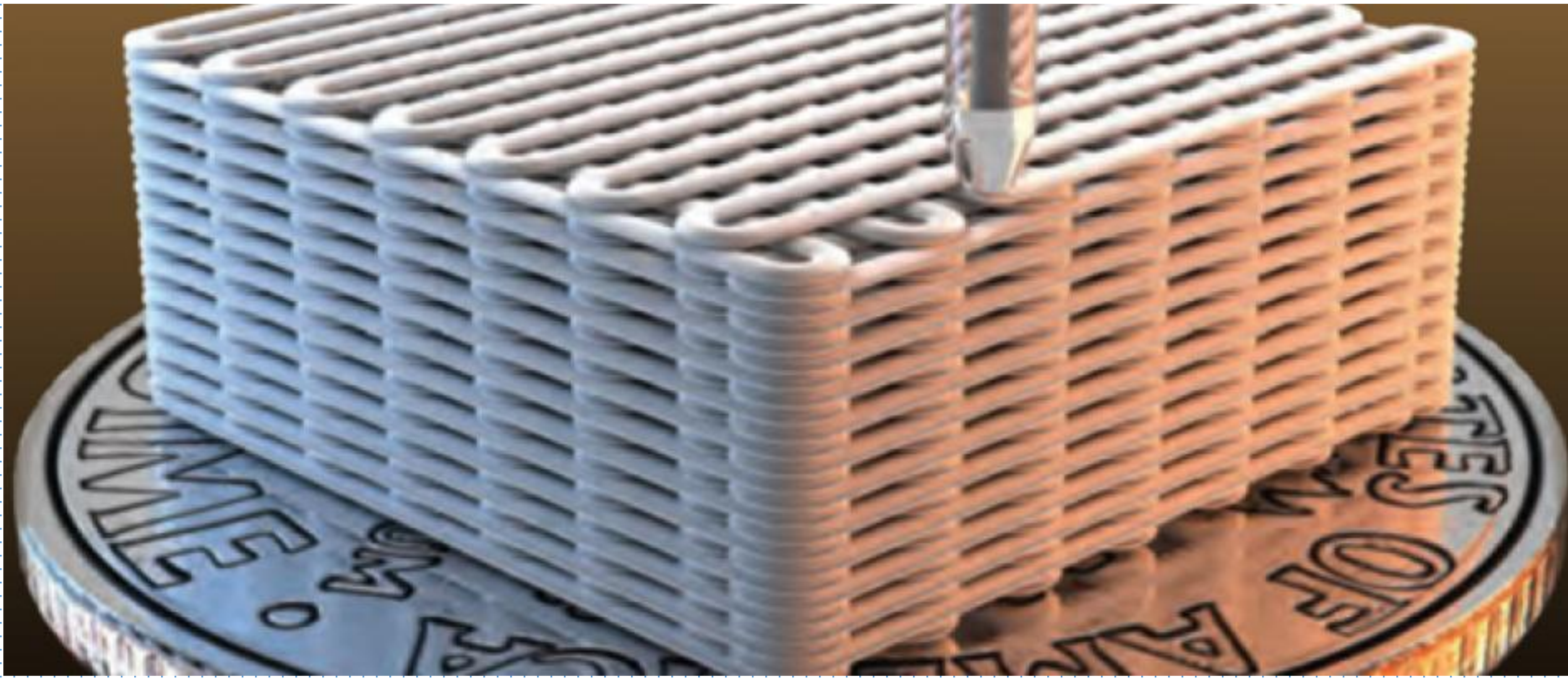
Since the launch of MGI in 2011, the Federal government has invested over $250 million in new R&D and innovation infrastructure to anchor the use of advanced materials in existing and emerging industrial sectors in the United States.

Materials Genome Initiative

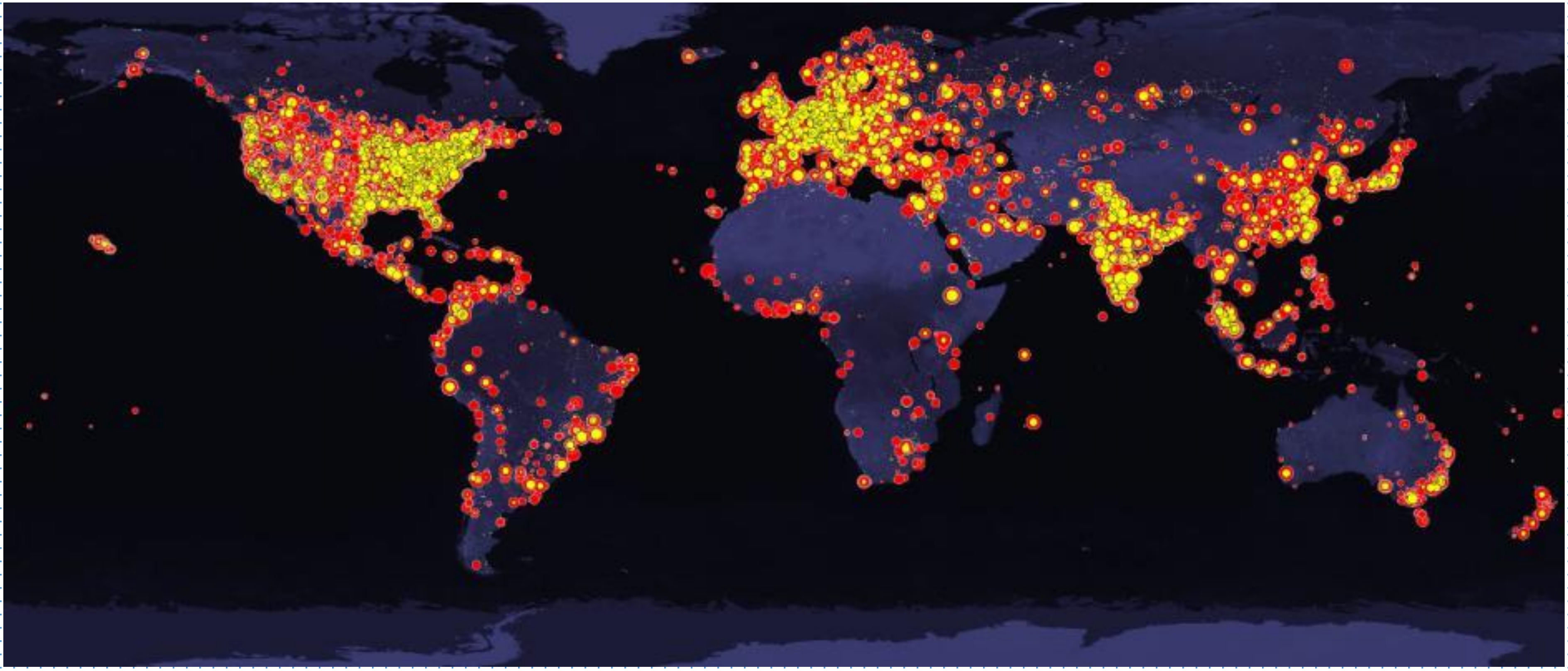


The development of a materials innovation infrastructure (MII) that will enable rapid and significant reductions in the development time for new materials with improved properties is a critical element of the Materials Genome Initiative (MGI).

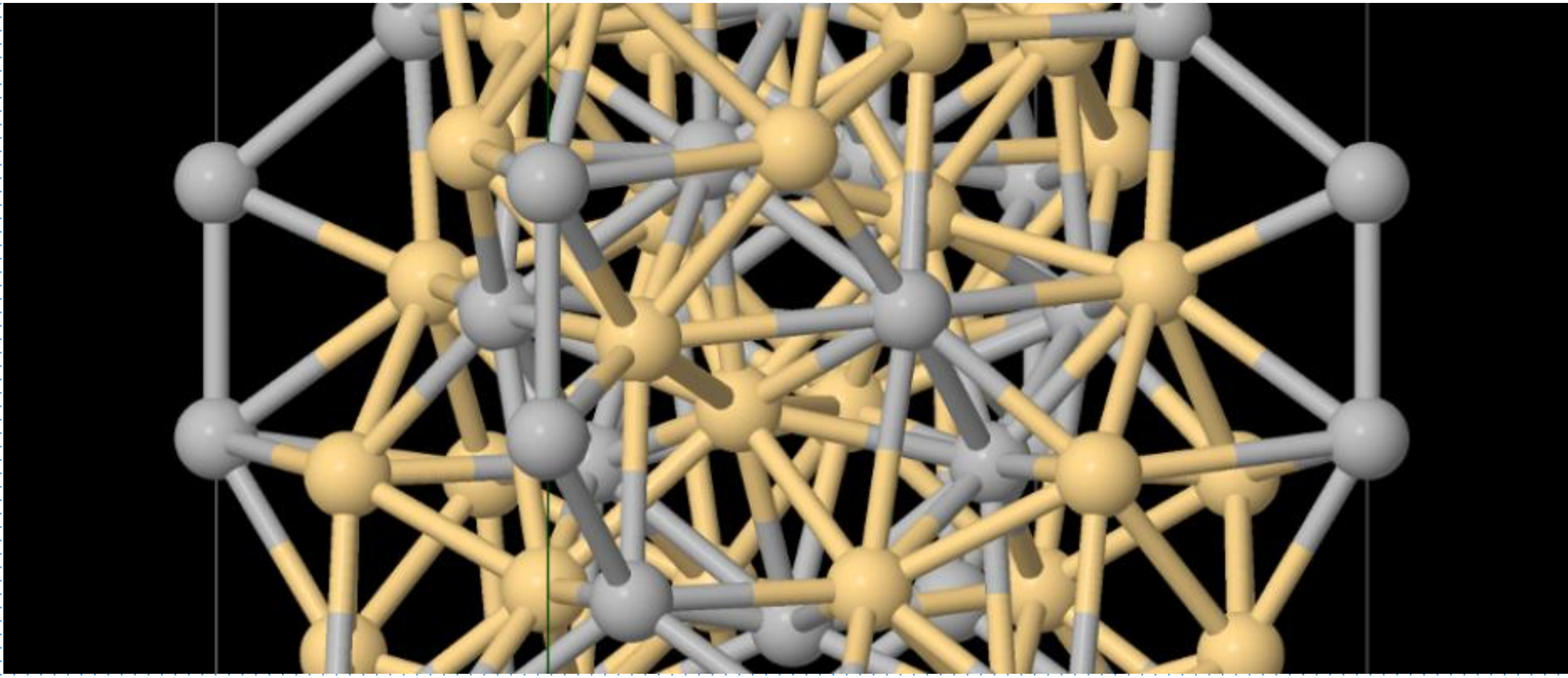
Materials Genome Initiative



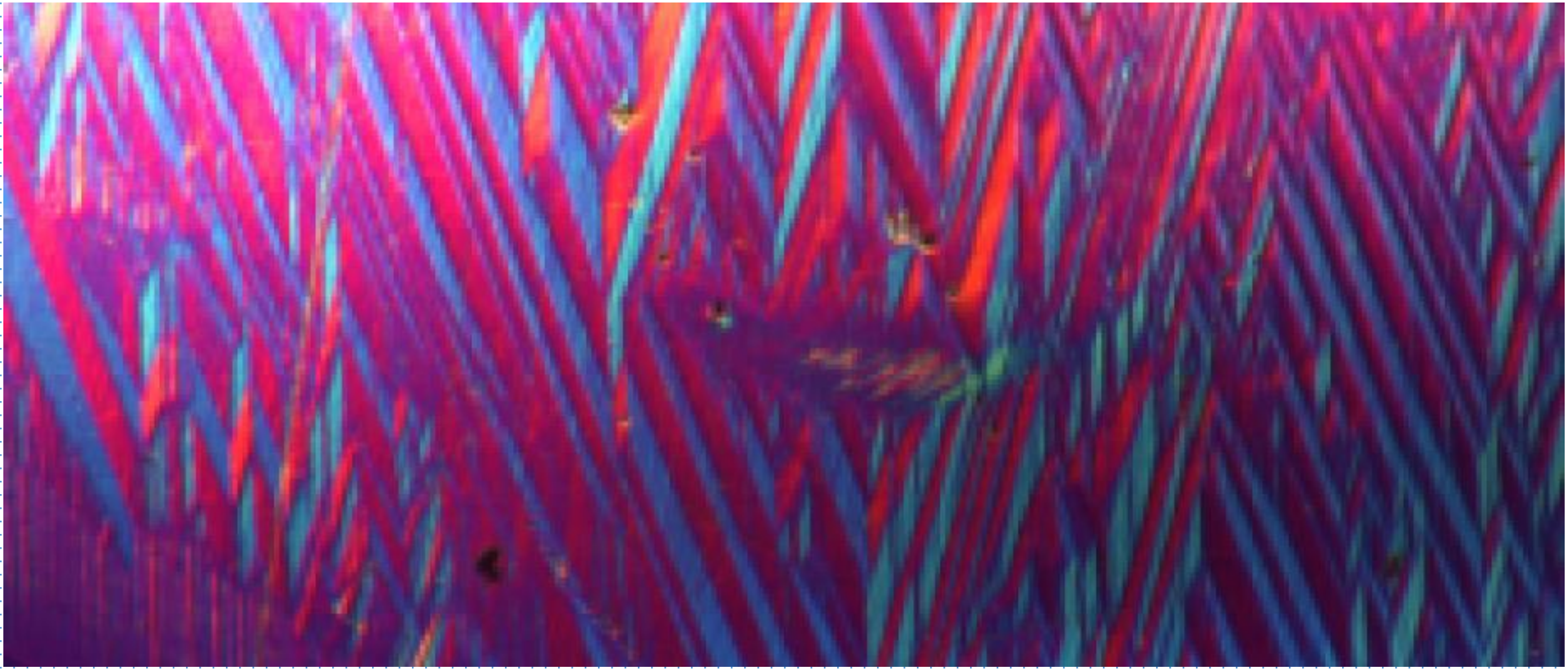
3-D printed graphene aerogels could improve sensors and batteries



Graphic Simulation of the 250,000 nanoHUB users worldwide.
Image courtesy 2014 MGI Strategic Plan.



Showcase material from the Automatic-FLOW for Materials Discovery.



Unusual microstructure of $Zn_{45}Au_{30}Cu_{25}$
with satisfaction of the cofactor conditions

PERIODIC TABLE OF THE ELEMENTS

Table of Selected Radioactive Isotopes

1/IA	2/IIA	3/IIIA	4/IVA	5/VA	6/VIA	7/VIIA	8	9 VIIIA	10	11/IB	12/IIB	13/IIIB	14/IVB	15/VB	16/VIB	17/VIIB	18/VIII
1 H 1.00794 Hydrogen																	2 He 4.00260 Helium
3 Li 6.941 Lithium	4 Be 9.01218 Beryllium											5 B 10.811 Boron	6 C 12.011 Carbon	7 N 14.0067 Nitrogen	8 O 15.9994 Oxygen	9 F 18.998403 Fluorine	10 Ne 20.1797 Neon
11 Na 22.98977 Sodium	12 Mg 24.305 Magnesium											13 Al 26.98154 Aluminum	14 Si 28.0855 Silicon	15 P 30.97376 Phosphorus	16 S 32.066 Sulfur	17 Cl 35.4527 Chlorine	18 Ar 39.948 Argon
19 K 39.0983 Potassium	20 Ca 40.078 Calcium	21 Sc 44.9559 Scandium	22 Ti 47.87 Titanium	23 V 50.9415 Vanadium	24 Cr 51.996 Chromium	25 Mn 54.9380 Manganese	26 Fe 55.845 Iron	27 Co 58.9332 Cobalt	28 Ni 58.6934 Nickel	29 Cu 63.546 Copper	30 Zn 65.39 Zinc	31 Ga 69.723 Gallium	32 Ge 72.61 Germanium	33 As 74.9216 Arsenic	34 Se 78.96 Selenium	35 Br 79.904 Bromine	36 Kr 83.80 Krypton
37 Rb 85.4678 Rubidium	38 Sr 87.62 Strontium	39 Y 88.9059 Yttrium	40 Zr 91.224 Zirconium	41 Nb 92.9064 Niobium	42 Mo 95.94 Molybdenum	43 Tc (98) Technetium	44 Ru 101.07 Ruthenium	45 Rh 102.9055 Rhodium	46 Pd 106.42 Palladium	47 Ag 107.868 Silver	48 Cd 112.41 Cadmium	49 In 114.82 Indium	50 Sn 118.710 Tin	51 Sb 121.760 Antimony	52 Te 127.60 Tellurium	53 I 126.9045 Iodine	54 Xe 131.29 Xenon
55 Cs 132.9054 Cesium	56 Ba 137.33 Barium	57 La* 138.9055 Lanthanum	72 Hf 178.49 Hafnium	73 Ta 180.9479 Tantalum	74 W 183.84 Tungsten	75 Re 186.207 Rhenium	76 Os 190.23 Osmium	77 Ir 192.22 Iridium	78 Pt 195.08 Platinum	79 Au 196.9665 Gold	80 Hg 200.59 Mercury	81 Tl 204.383 Thallium	82 Pb 207.2 Lead	83 Bi 208.9804 Bismuth	84 Po (209) Polonium	85 At (210) Astatine	86 Rn (222) Radon
87 Fr (223) Francium	88 Ra (226) Radium	89 Ac** (227) Actinium	104 Rf (261) Rutherfordium	105 Db (262) Dubnium	106 Sg (263) Seaborgium	107 Bh (264) Bohrium	108 Hs (265) Hassium	109 Mt (268) Meitnerium	110 Uun (269) (Ununnilium)	111 Uuu (272) (Unununium)	112 Uub (277) (Ununbium)	113 (Ununtrium)	114 Uuq (285) (Ununquadium)	115 (Ununpentium)	116 (Ununhexium)	117 (Ununseptium)	118 (Ununoctium)

* Estimated Values

*	58 Ce 140.12 Cerium	59 Pr 140.9077 Praseodymium	60 Nd 144.24 Neodymium	61 Pm (145) Promethium	62 Sm 150.36 Samarium	63 Eu 151.964 Europium	64 Gd 157.25 Gadolinium	65 Tb 158.9253 Terbium	66 Dy 162.50 Dysprosium	67 Ho 164.9303 Holmium	68 Er 167.26 Erbium	69 Tm 168.9342 Thulium	70 Yb 173.04 Ytterbium	71 Lu 174.967 Lutetium
**	90 Th 232.0381 Thorium	91 Pa 231.0359 Protactinium	92 U 238.029 Uranium	93 Np (237) Neptunium	94 Pu (244) Plutonium	95 Am (243) Americium	96 Cm (247) Curium	97 Bk (247) Berkelium	98 Cf (251) Californium	99 Es (252) Einsteinium	100 Fm (257) Fermium	101 Md (258) Mendelevium	102 No (259) Nobelium	103 Lr (262) Lawrencium

KEY: ATOMIC NUMBER; ATOMIC WEIGHT (2); OXIDATION STATES (Bold most stable); BOILING POINT, K; MELTING POINT, K; SYMBOL; DENSITY at 300 K (3) (g/cm³); ELECTRON CONFIGURATION; NAME

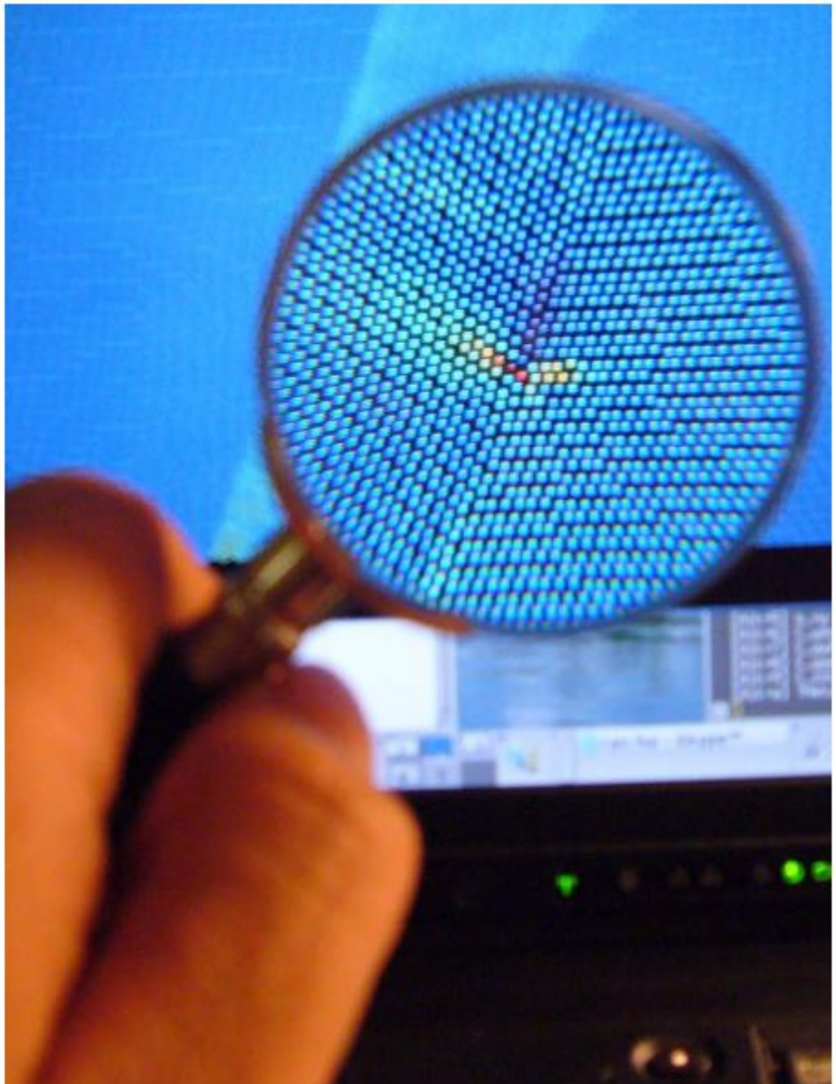
30 Zn 65.39 — 1180, 692.73, 7.13, [Ar]3d¹⁰4s², Zinc

NOTES:
(1) Black — solid. Red — gas. Blue — liquid.
(2) Based upon carbon-12. ( ) indicates most stable or best known isotope.
(3) Entries marked with daggers refer to the ...

The A & B subgroup designations, are those recommended by the International Union of Pure and Applied Chemistry.

Sargent-Welch

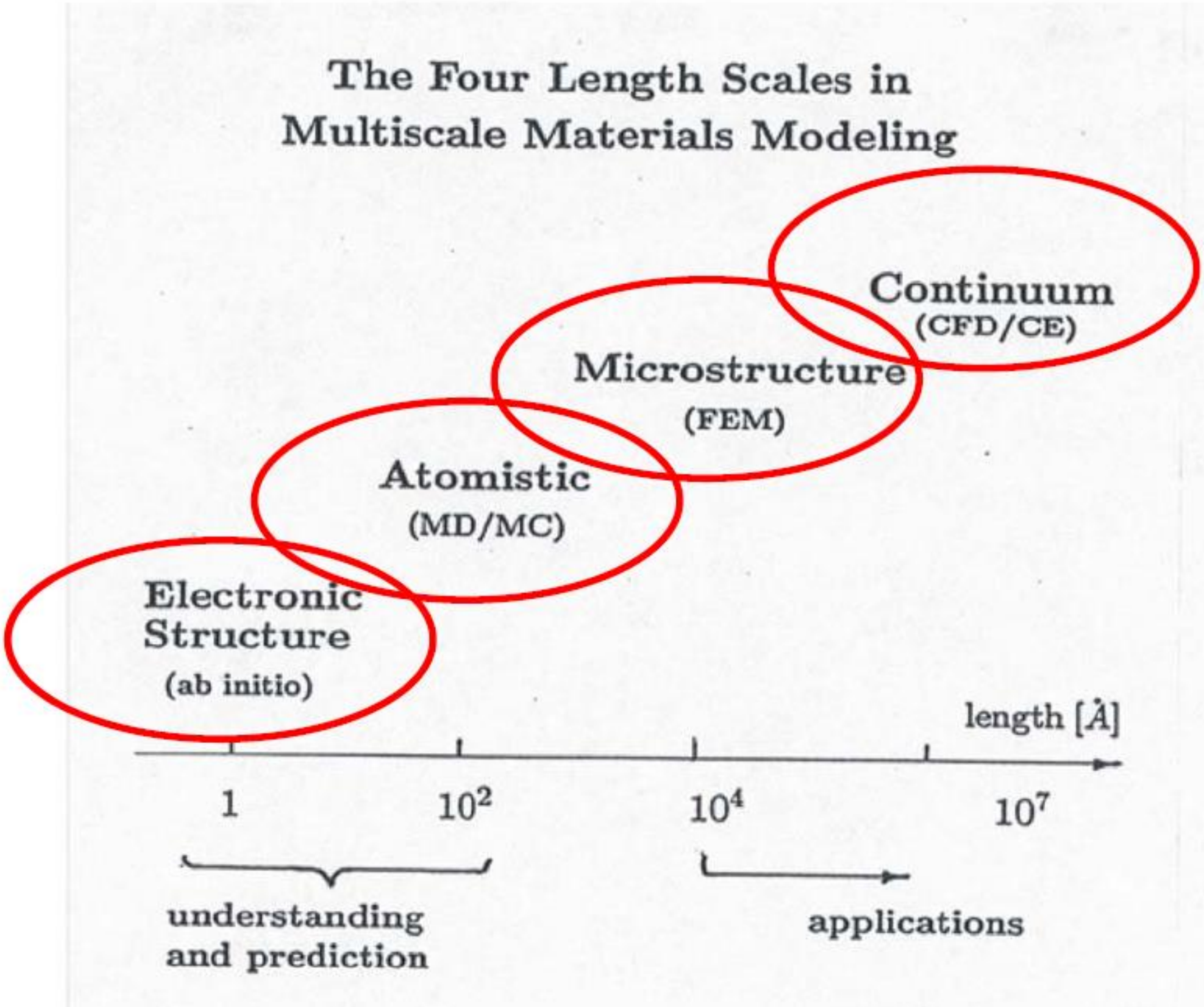
Atomistic modelling —
molecular dynamics (MD) methods



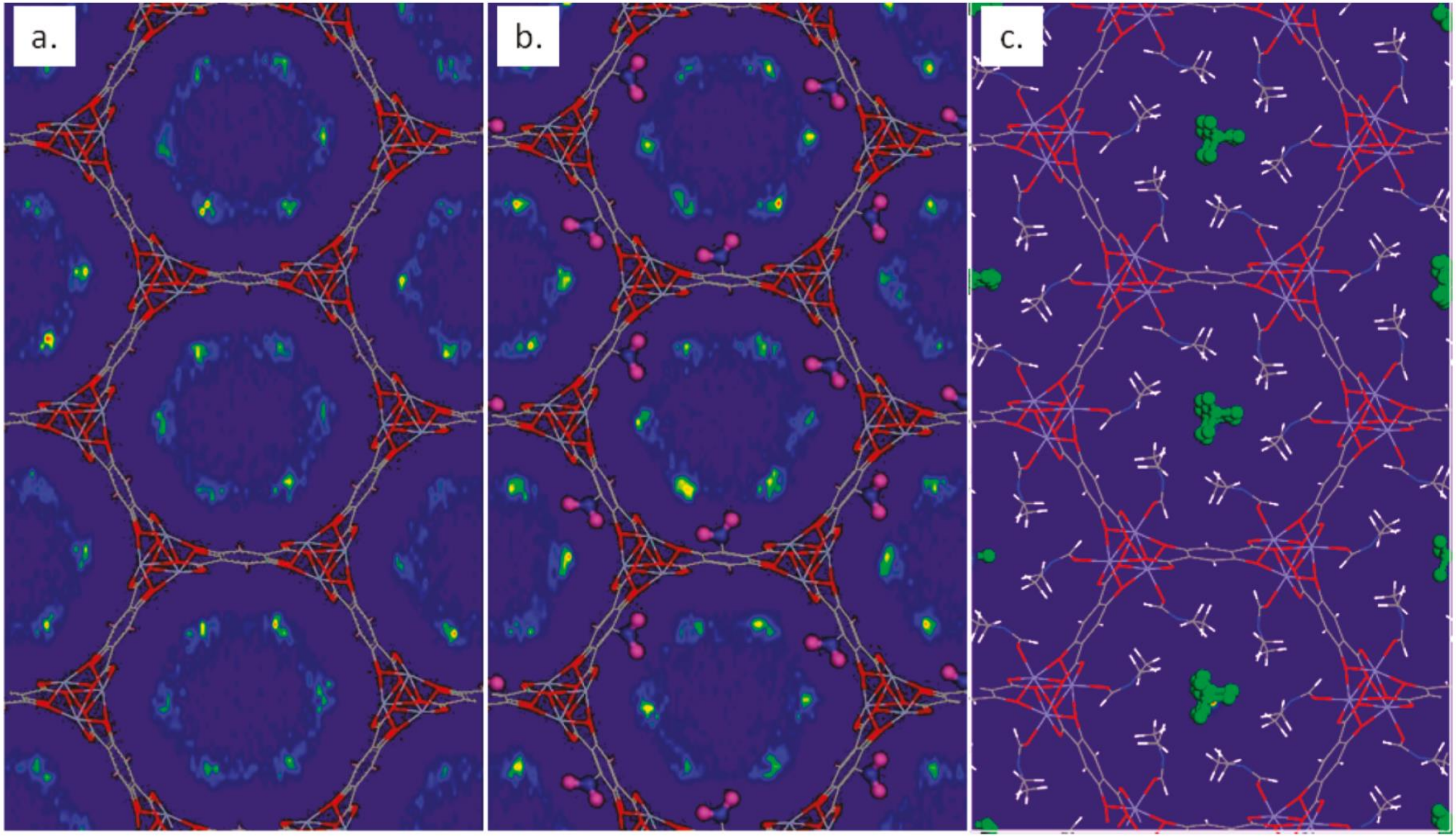
MD simulation

Observing and measuring
atoms in a virtual lab

The Secret Life Of
Your Atoms



Material science → Engineering



Probability density plots in the xy plane of methane adsorption in Zn_2(dhtp) Zn_2(dhtp)-NH_2 Zn_2(dhtp)-DMF