

# Discovering Materials Using the Highway Lane

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# THE U.S. MATERIALS GENOME INITIATIVE

*“...to discover, develop, and deploy new materials twice as fast, we’re launching what we call the Materials Genome Initiative”*

—President Obama, 2011

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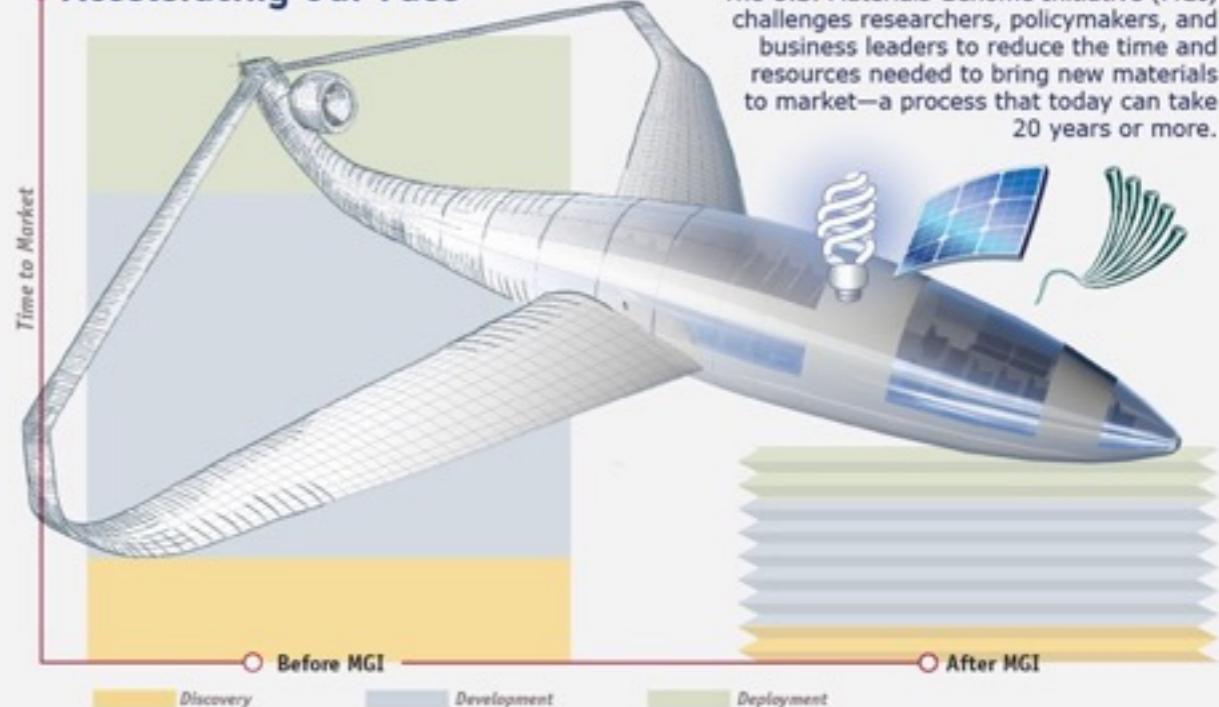
*President Obama, 2011*

## Meeting Societal Needs

Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.



## Accelerating Our Pace



## Building Infrastructure for Success

The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.

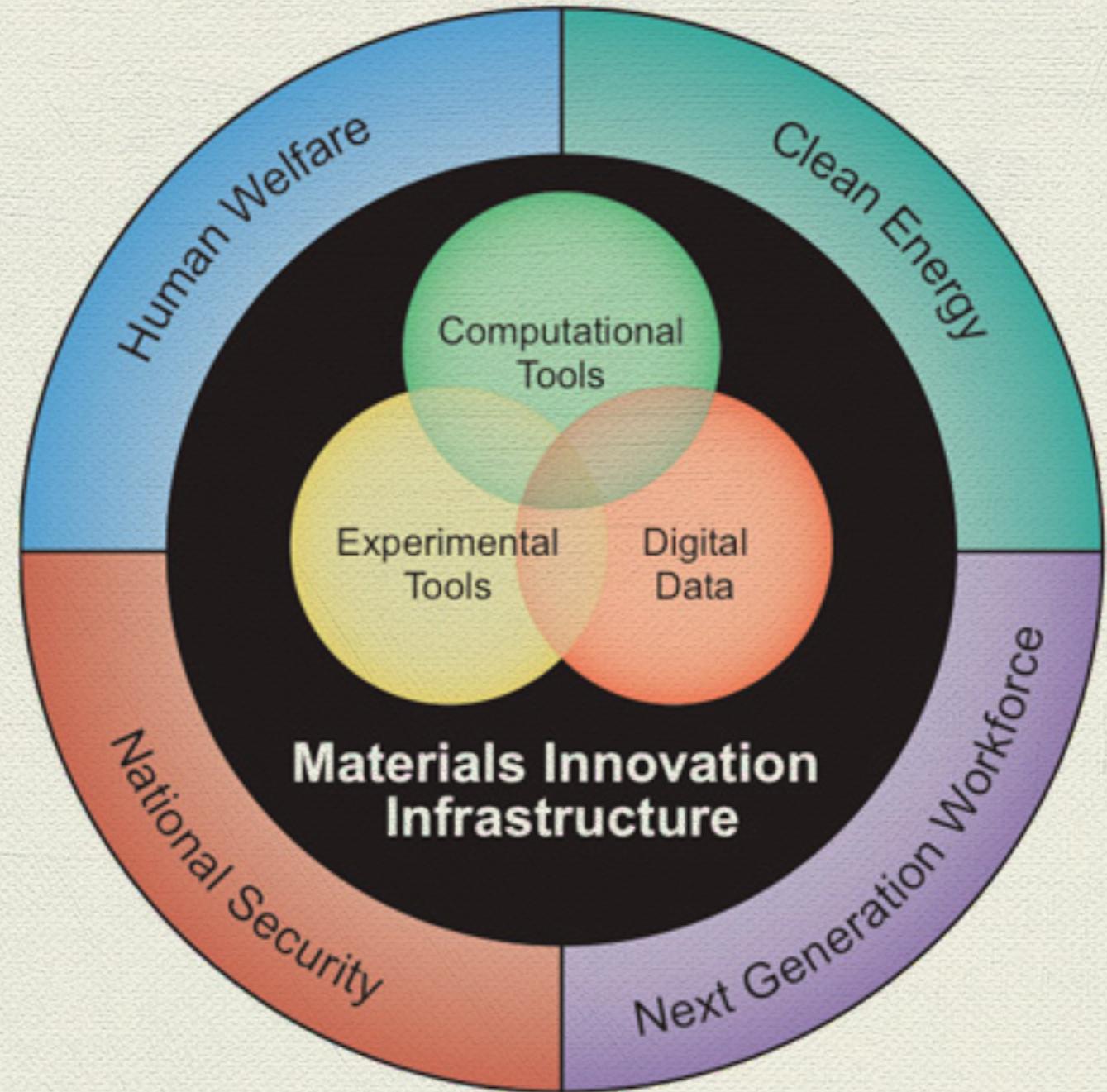


*...yet the time lag between discovery of advanced materials and their use in commercial products can be 20 years or more.*

*MGI Strategic Plan (Dec 2014)*

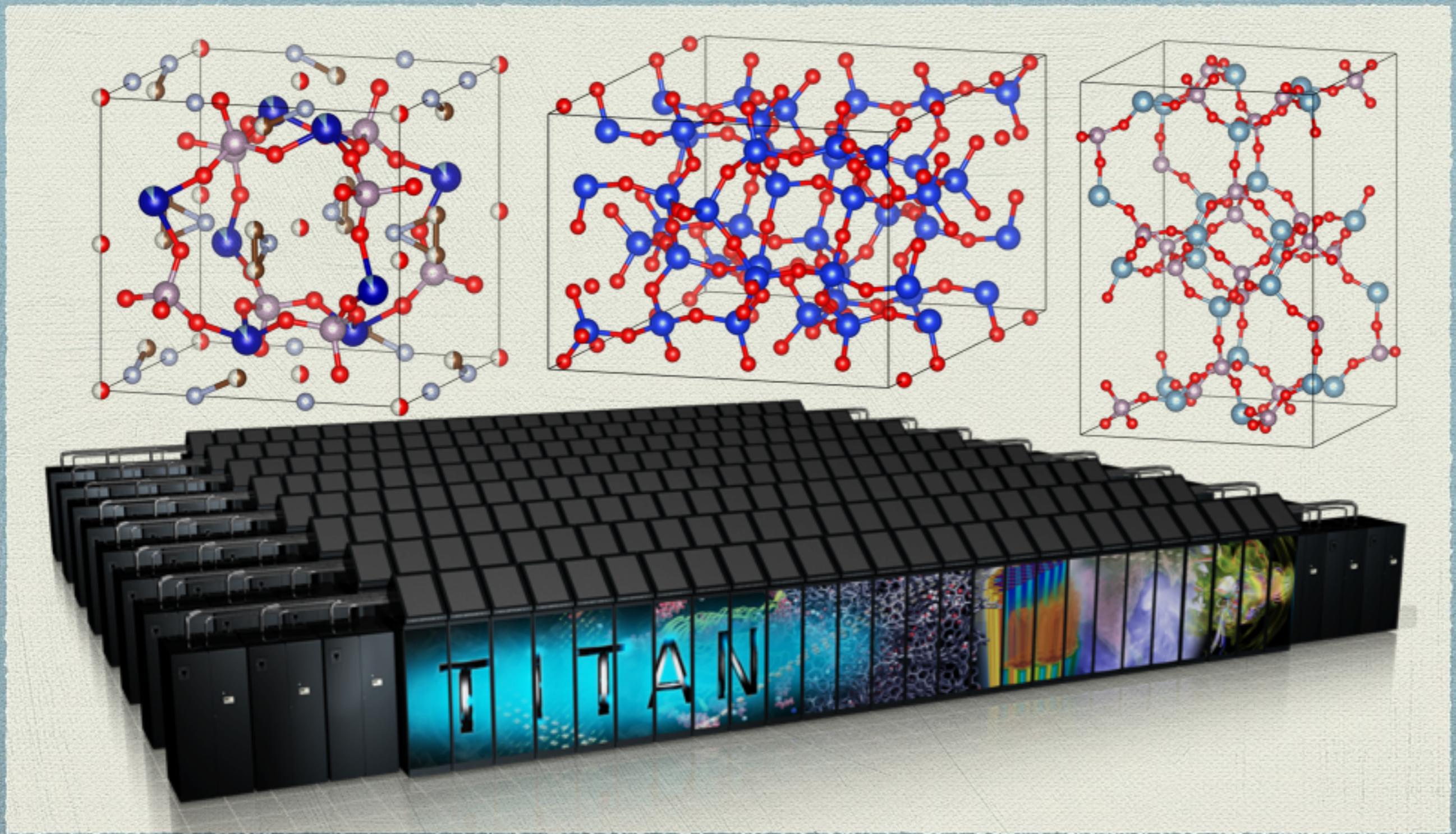
*...to help businesses  
discover, develop, and  
deploy new materials  
twice as fast.*

*MGI Strategic Plan  
(Dec 2014)*

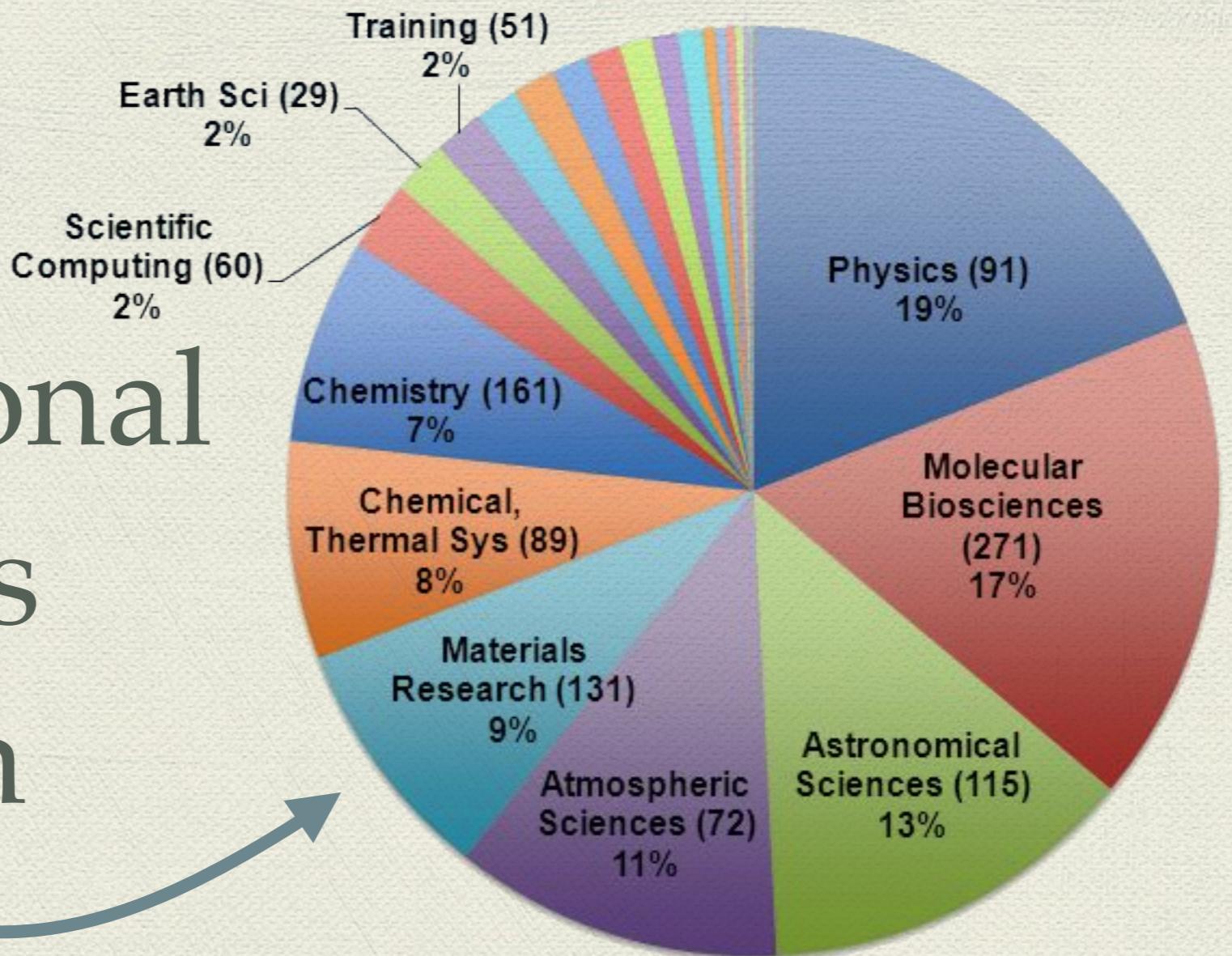


*A \$250 million research investment by DOE, NSF, and NIST  
Anticipated 10-fold increase over the next decade.  
<https://www.whitehouse.gov/mgi/goals>*

# High-throughput materials discovery



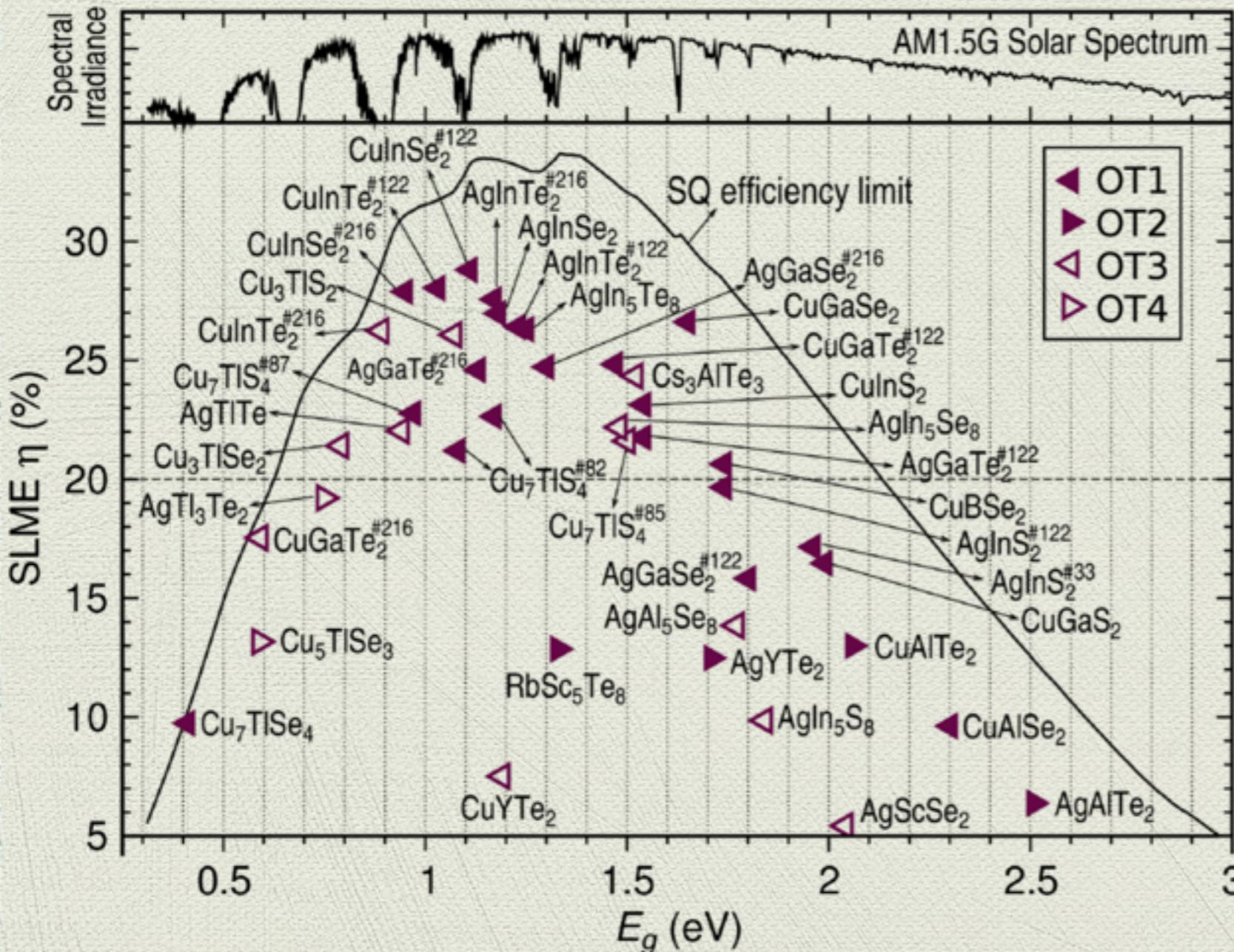
# Computational Materials Research



According to XSede usage (2015)

# HTC for Energy Materials

## Photovoltaics: HT screening of light-absorbing materials.

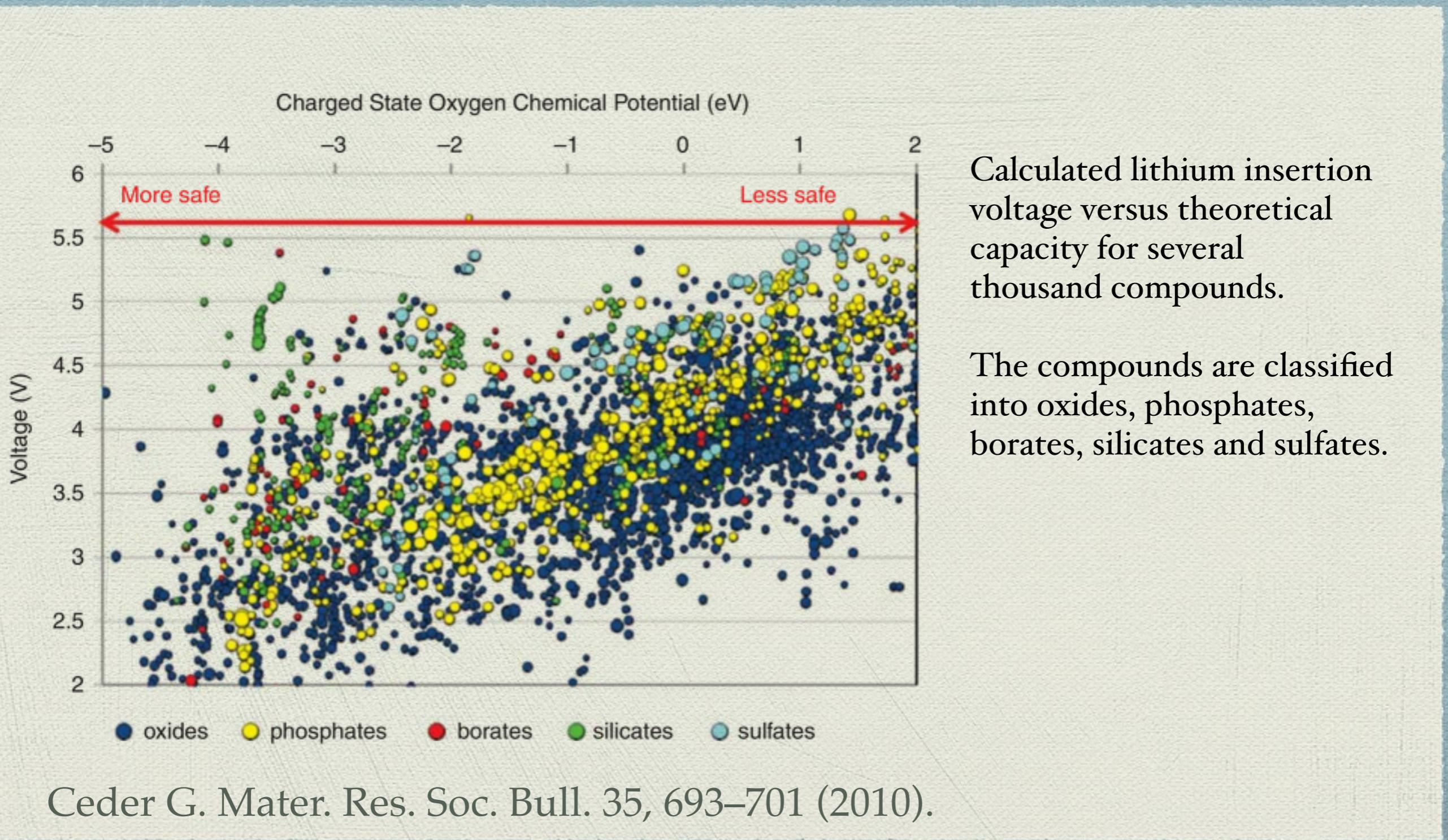


Spectroscopic limited maximum efficiency (SLME) versus the minimum gap ( $E_g$ ) for generalized I–III–VI chalcopyrite materials identified as having a high SLME.

All of the currently used PV absorbers were found as well as new materials with promising values (with SLME > 20%).

# HTC for Energy Materials

## Li-ion batteries: HT calculations of charge capacity vs Voltage



# Au nanoparticles on Anatase ( $\text{TiO}_2$ )



DOI: 10.1021/acs.jpclett.5b00655

Letter

[pubs.acs.org/JPCL](http://pubs.acs.org/JPCL)

## **Design and Preparation of Supported Au Catalyst with Enhanced Catalytic Activities by Rationally Positioning Au Nanoparticles on Anatase**

Liang Wang,<sup>‡</sup> Hong Wang,<sup>\*,†</sup> Andrew E. Rice,<sup>†</sup> Wei Zhang,<sup>\*,§</sup> Xiaokun Li,<sup>||</sup> Mingshu Chen,<sup>||</sup> Xiangju Meng,<sup>‡</sup> James P. Lewis,<sup>†</sup> and Feng-Shou Xiao<sup>\*,‡</sup>

... we have developed an efficient way to boost the activity of Au nanocatalysts. Coupling computational models with synthesis and characterization, the cooperation between Au and anatase is significantly enhanced by rationally positioning the Au nanoparticles on the edged/corner sites.

... Au nanoparticles positioned on the edge/corner sites of  $\text{TiO}_2$  supports offers an excellent opportunity for designing and developing highly “controlled” catalysts in the future.

# Nitroarene Hydrogenation



DOI: 10.1021/acscatal.6b00530

Research Article

pubs.acs.org/acscatalysis

## Activity and Selectivity in Nitroarene Hydrogenation over Au Nanoparticles on the Edge/Corner of Anatase

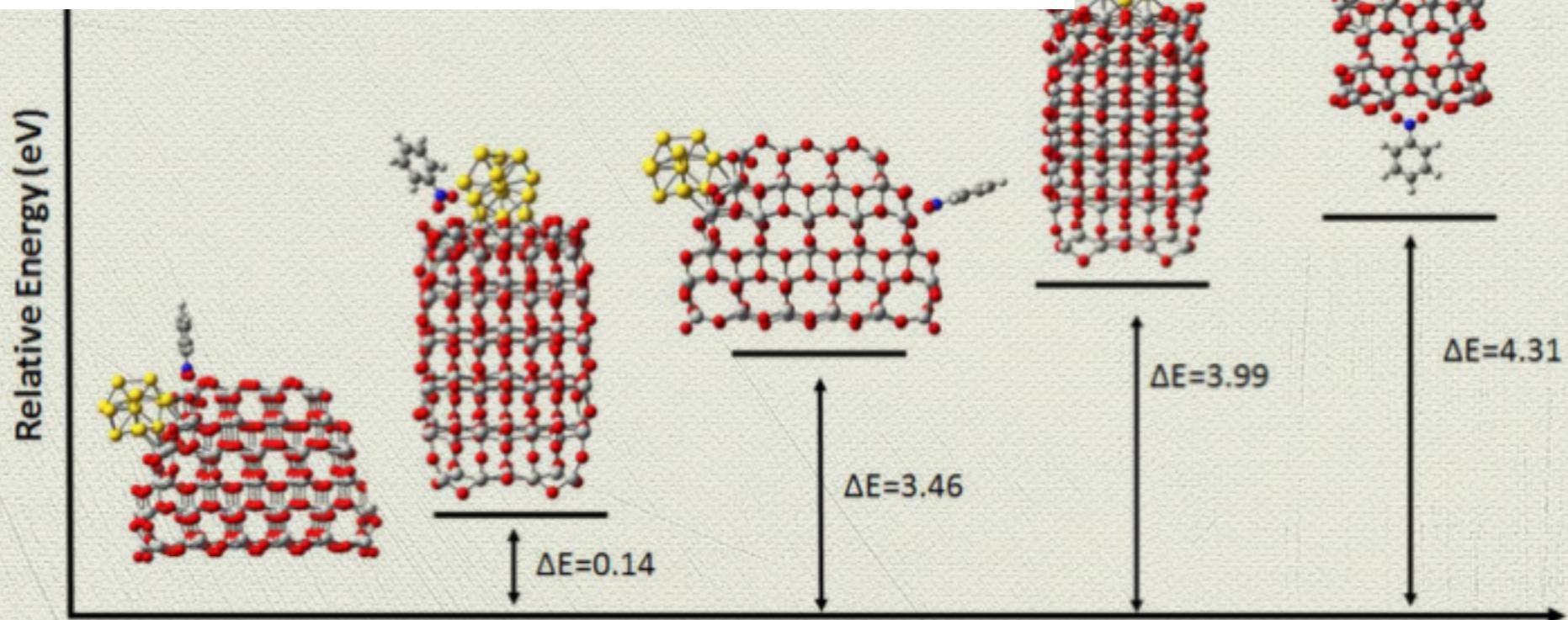
Liang Wang <sup>\*,†</sup>, Jian Zhang, <sup>†</sup> Hong Wang, <sup>\*,‡</sup> Yi Shao, <sup>§</sup> Xiaohui Liu, <sup>§</sup> Yan-Qin Wang, <sup>§</sup> James P. Lewis, <sup>‡</sup> and Feng-Shou Xiao <sup>\*,†,||</sup>

<sup>†</sup>Key Lab of Applied Chemistry of Zhejiang Province, Department of Chemistry, Zhejiang University, Hangzhou 310028, China

<sup>‡</sup>Department of Physics and Astronomy, West Virginia University, Morgantown West Virginia 26506-6315, United States

<sup>§</sup>Institute of Catalysis, East China University of Science and Technology, Shanghai 200237, China

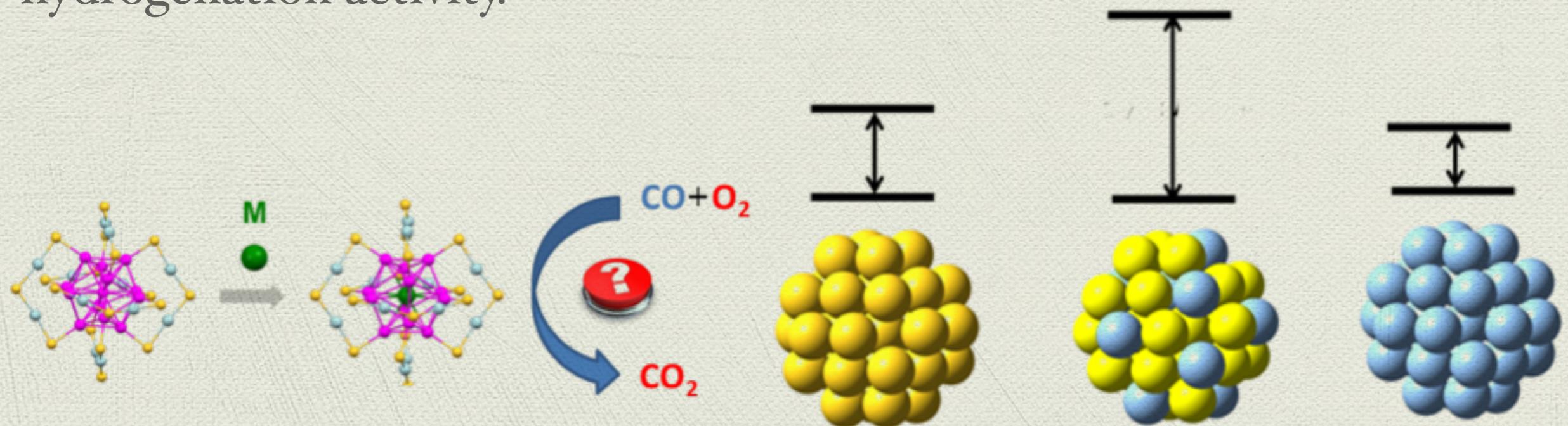
<sup>||</sup>Key Lab of Biomass Chemical Engineering of Ministry of Education, Zhejiang University, Hangzhou 310027, China



# Bi-metallic nanoparticles

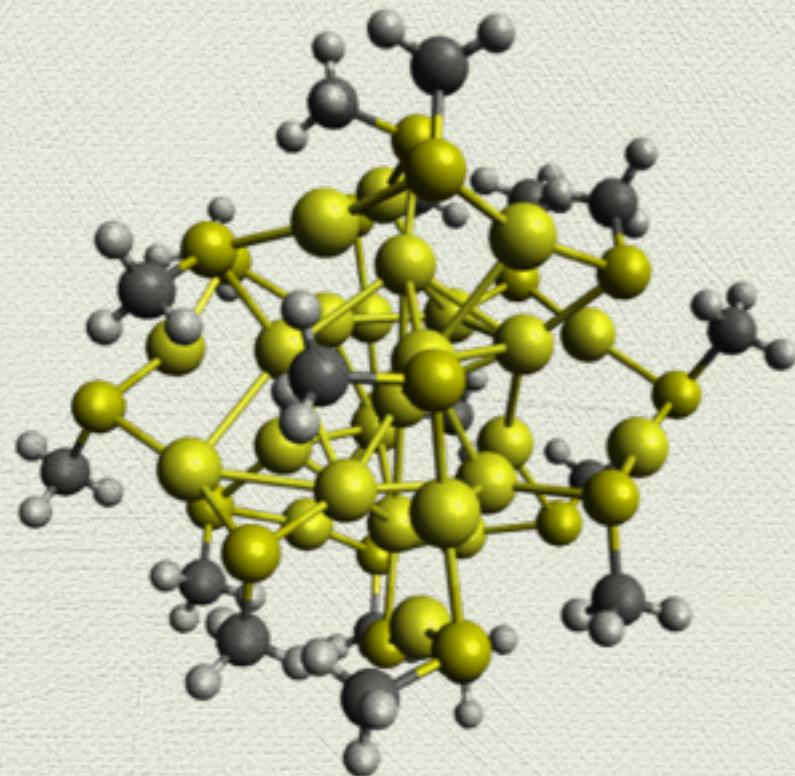
Catalytic activity is enhanced by a smart combination of transition metals compare to the activity of their precursors. Doping center atom will significantly change catalytic properties

Hg, Ag doping both suppress CO oxidation, but enhance hydrogenation activity.



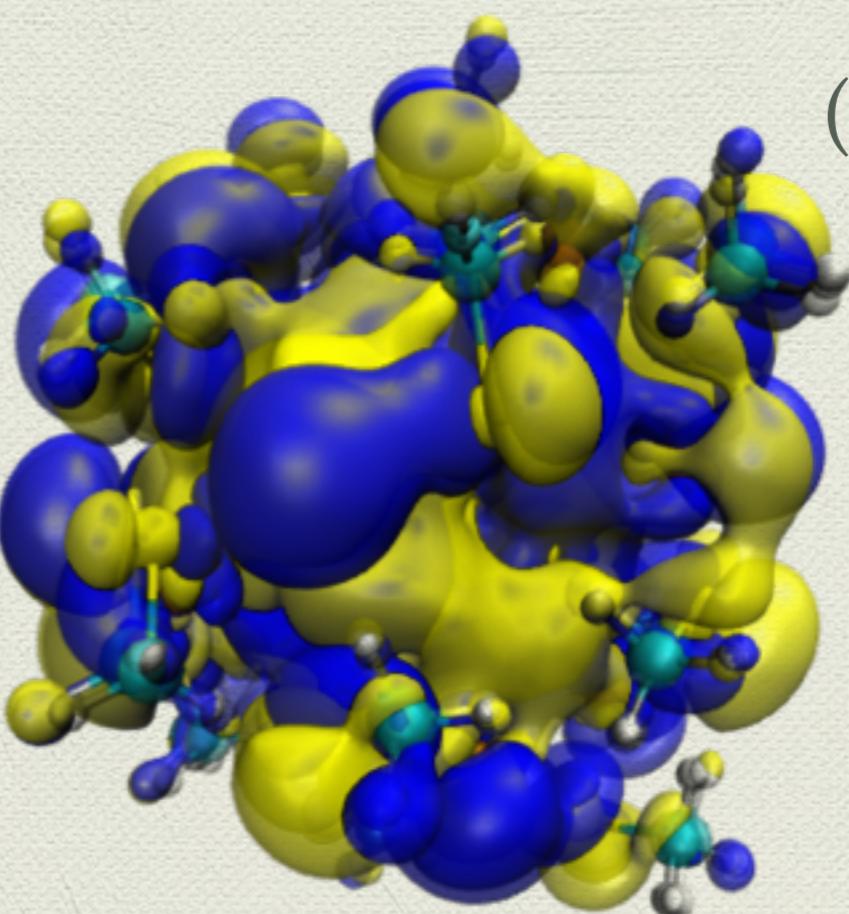
CO and CO<sub>2</sub> conversion and biomass hydrogenation

# Bi-metallic nanoparticles



$\text{Au}_{25}(\text{SCH}_3)_{18}$

Undoped



Ag Doped  
(outer) (inner)

# Zeolites



DOI: 10.1021/jacs.6b04951

Communication

[pubs.acs.org/JACS](http://pubs.acs.org/JACS)

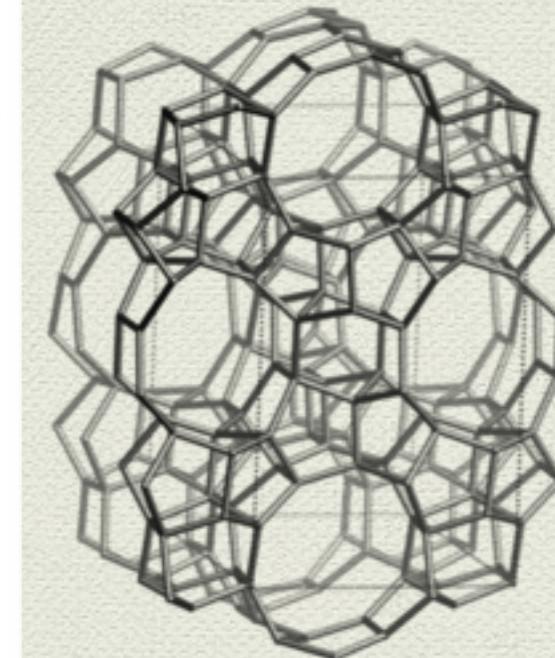
## Product Selectivity Controlled by Zeolite Crystals in Biomass Hydrogenation over a Palladium Catalyst

Chengtao Wang,<sup>†</sup> Liang Wang,<sup>\*,†</sup> Jian Zhang,<sup>†</sup> Hong Wang,<sup>‡</sup> James P. Lewis,<sup>‡</sup> and Feng-Shou Xiao<sup>\*,†,§</sup>

<sup>†</sup>Key Lab of Applied Chemistry of Zhejiang Province, Department of Chemistry, Zhejiang University, Hangzhou 310028, China

<sup>‡</sup>Department of Physics, West Virginia University, Morgantown, West Virginia 26506-6315, United States

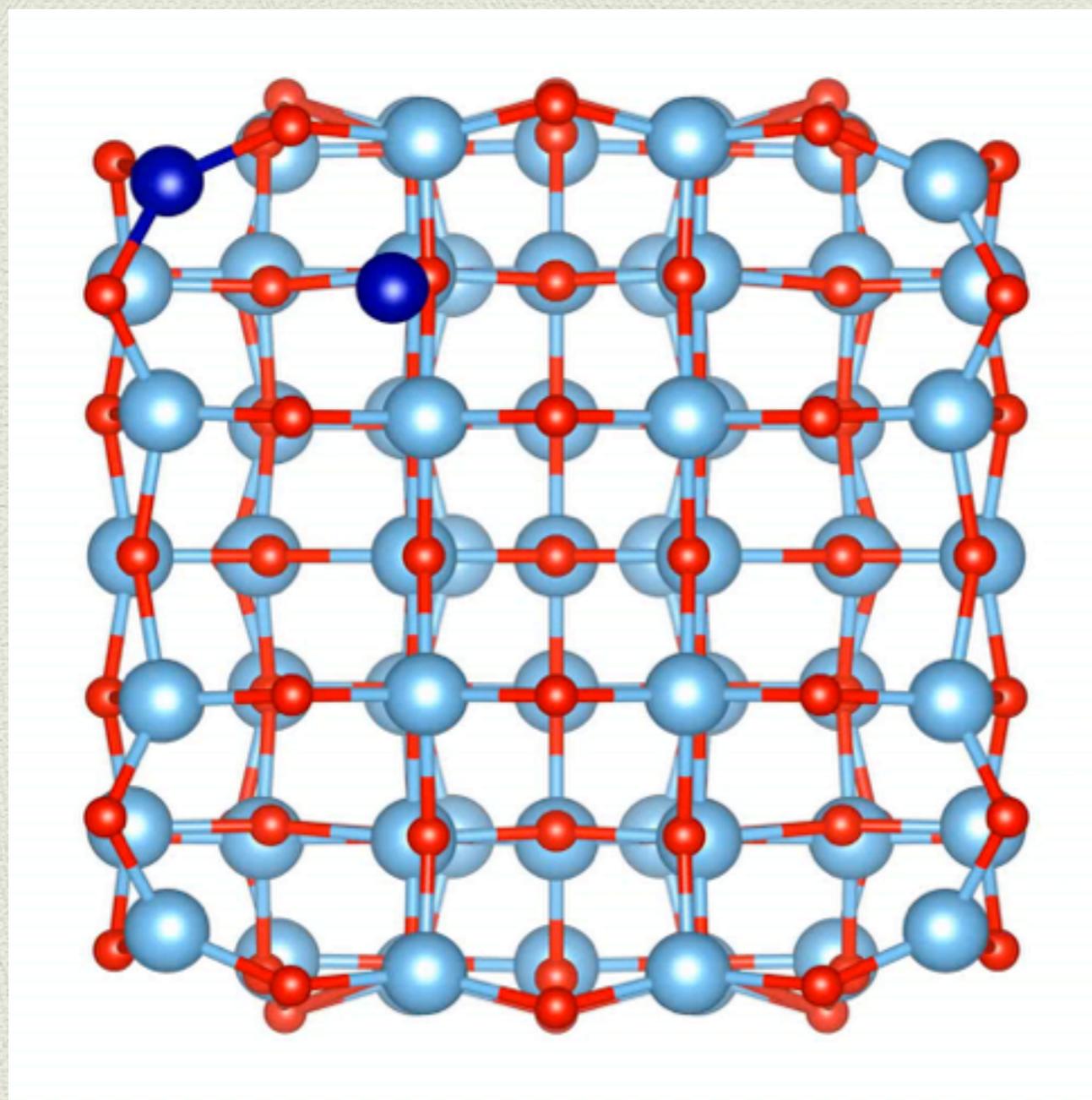
<sup>§</sup>Key Lab of Biomass Chemical Engineering of Ministry of Education, Zhejiang University, Hangzhou 310027, China



The key to this success is to combine the advantages of both Pd nanoparticles (highly active sites) and zeolite micropores (controllable diffusion of reactants and products).

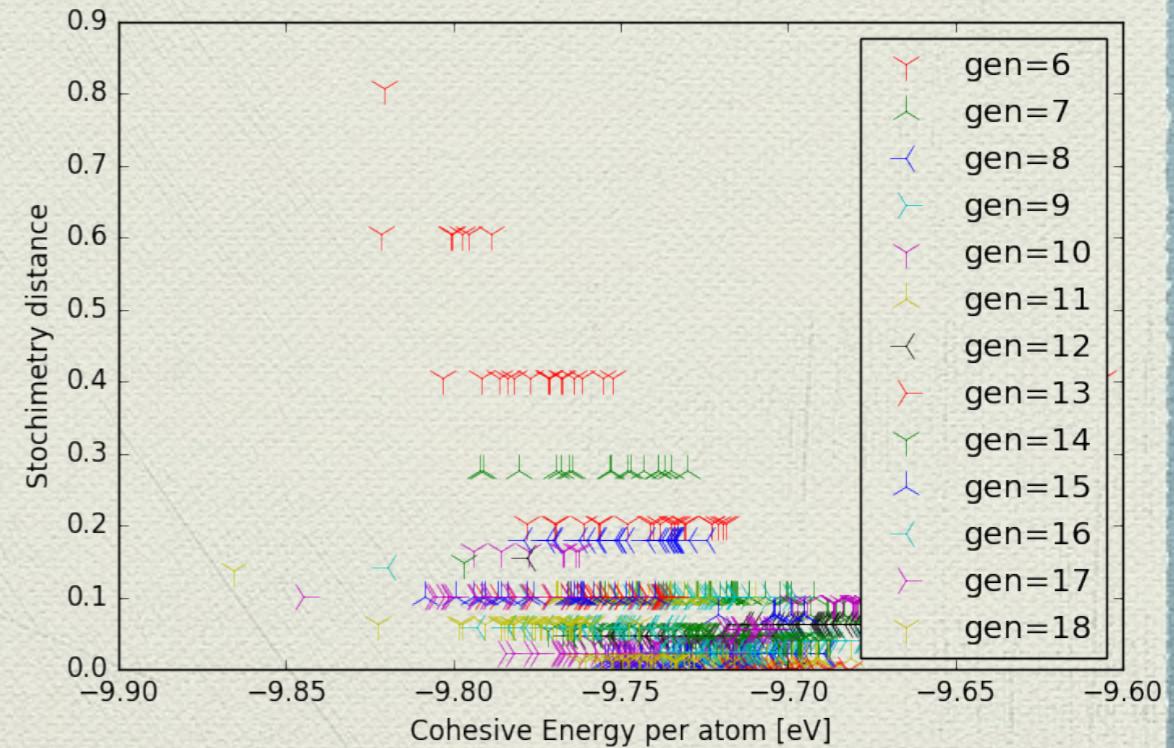
In the hydrogenation of biomass-derived furfural, the furan selectivity over the Pd@S-I is as high as 98.7%, outperforming the furan selectivity (5.6%) over conventional Pd nanoparticles impregnated with S-I zeolite crystals (Pd/S-I).

# $\text{C}_3\text{O}_4$ cluster growing on $\text{TiO}_2$



Cluster growing simulation using a tree search algorithm and a double stoichiometry and energy selectivity.

308 atoms for  $\text{TiO}_2$



# Funding

DOE Basic Energy Science – Program for Computational and Theoretical Chemistry

Designing Materials to Revolutionize and Engineer Our Future (with Rongchao Jin – CMU)

International Center of Excellence – Catalysis (with Prof. Feng-Shou Xiao – Zhejiang University)

3+ indirect patents



中科合成油技术有限公司  
SYNFUELS CHINA



# Fireball



**FIREBALL** is a suite of programs designed to perform calculations using ab initio tight-binding molecular dynamics, having favorable accuracy/efficiency balance Based on TB-DFT (Tight-Binding Density Functional Theory).

Fireball code is an efficient first-principles exploratory tool allowing to handle complex systems including thousands of atoms.

PHYSICAL REVIEW B

VOLUME 40, NUMBER 6

15 AUGUST 1989-II

## *Ab initio* multicenter tight-binding model for molecular-dynamics simulations and other applications in covalent systems

Otto F. Sankey and David J. Niklewski

Department of Physics, Arizona State University, Tempe, Arizona 85287-1504

(Received 21 February 1989)

PHYSICAL REVIEW B, VOLUME 64, 195103

## Further developments in the local-orbital density-functional-theory tight-binding method

James P. Lewis,<sup>1</sup> Kurt R. Glaesemann,<sup>1</sup> Gregory A. Voth,<sup>1</sup> Jürgen Fritsch,<sup>2</sup> Alexander A. Demkov,<sup>3</sup> José Ortega,<sup>4</sup> and Otto F. Sankey<sup>5</sup>

<sup>1</sup>Henry Eyring Center for Theoretical Chemistry and Department of Chemistry, University of Utah, 315 S. 1400 E., Rm. 2020, Salt Lake City, Utah 84112-0850

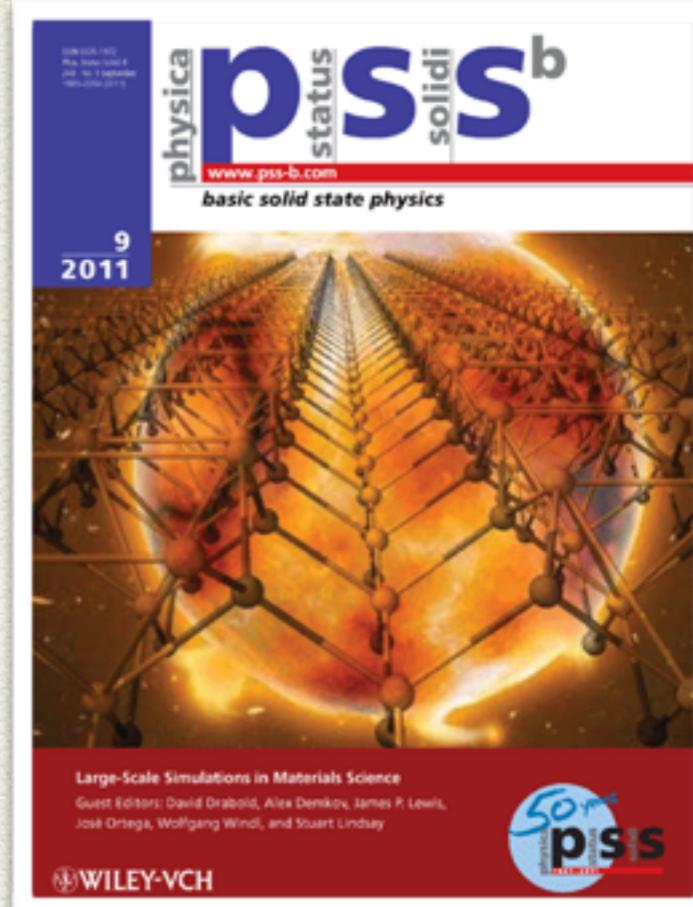
<sup>2</sup>Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

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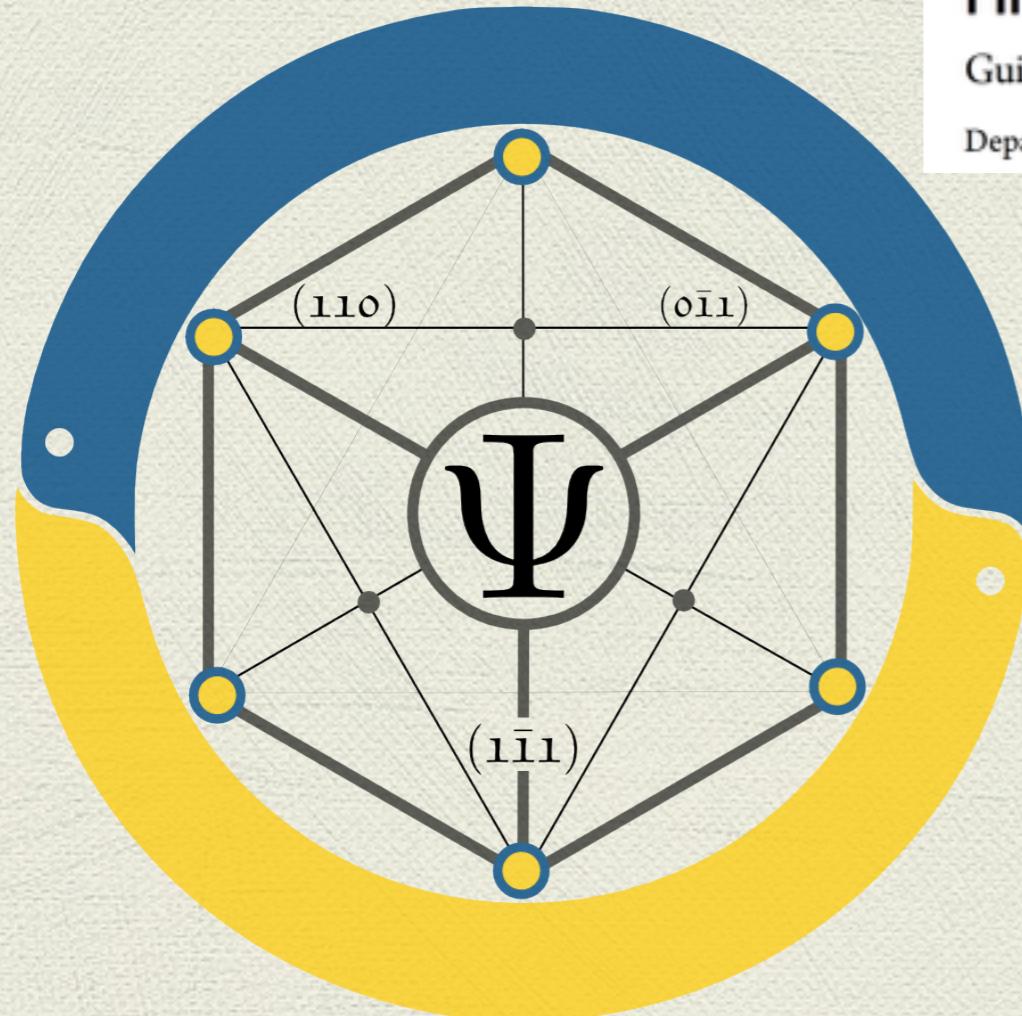
<sup>4</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

<sup>5</sup>Department of Physics and Astronomy, Arizona State University, Tempe, Arizona 85217-1504

(Received 22 December 2000; revised manuscript received 27 March 2001; published 15 October 2001)



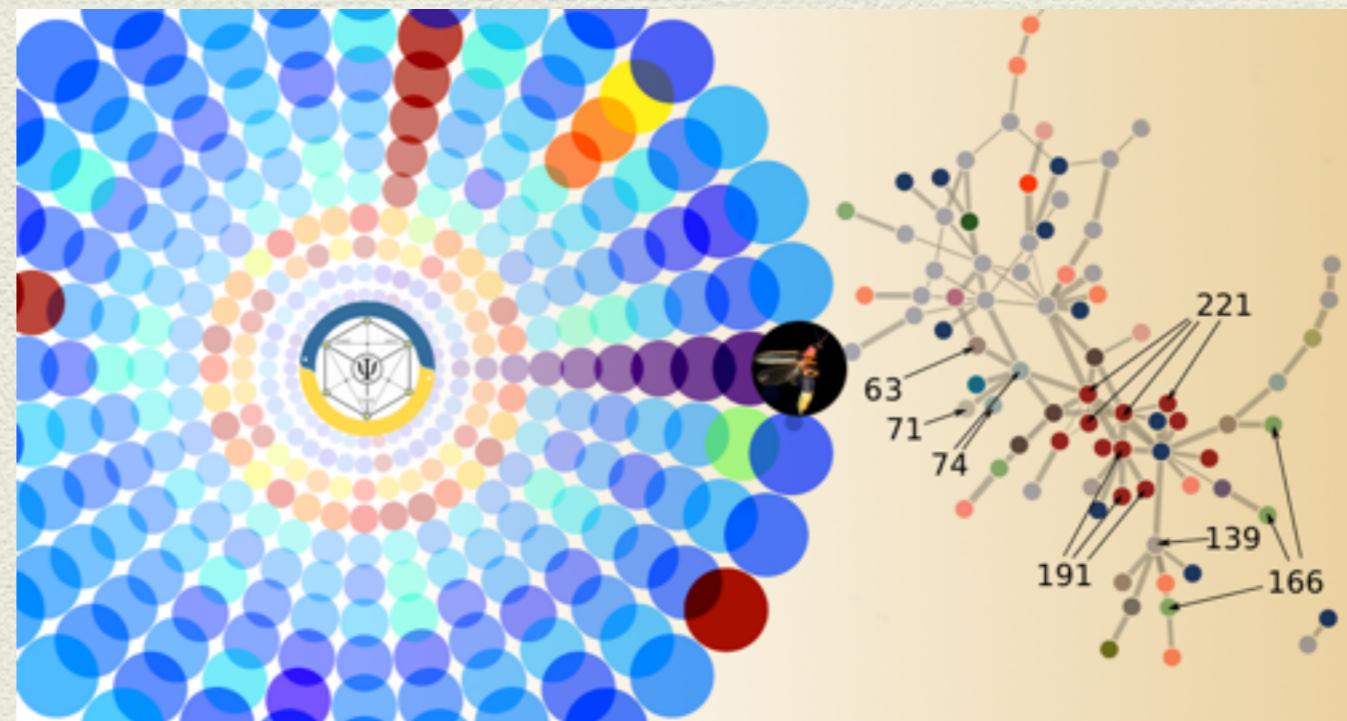
# PyChemia



## Firefly Algorithm for Structural Search

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Department of Physics and Astronomy, West Virginia University, Morgantown, West Virginia 26506, United States



PyChemia is an open-source Python library for High-throughput first-principles materials discovery. The focus of this library is on structural search and data analysis. The ultimate purpose of the code is to optimize the search of new materials using a variety of soft-computing-based and statistical methods.



# Conclusions

- ◆ Computers as a fast lane for materials discovery, cutting costs and time-to-market.
- ◆ We show some cases for energy materials.
- ◆ We present the several studies on the area of catalysis with metals on anatase, growing and optimization with bimetallics.
- ◆ The tools (Fireball, PyChemia) used for HT calculations for large numbers of atoms.
- ◆ Only HT methodologies can explore the diversity of catalytic processes and its optimization.

<https://github.com/fireball-dft/slides>

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*Thank you*