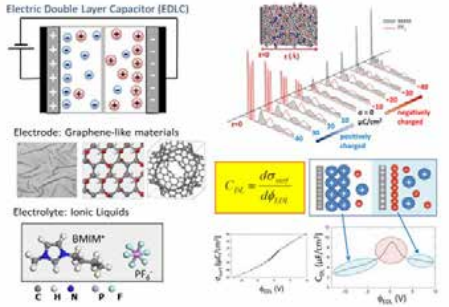
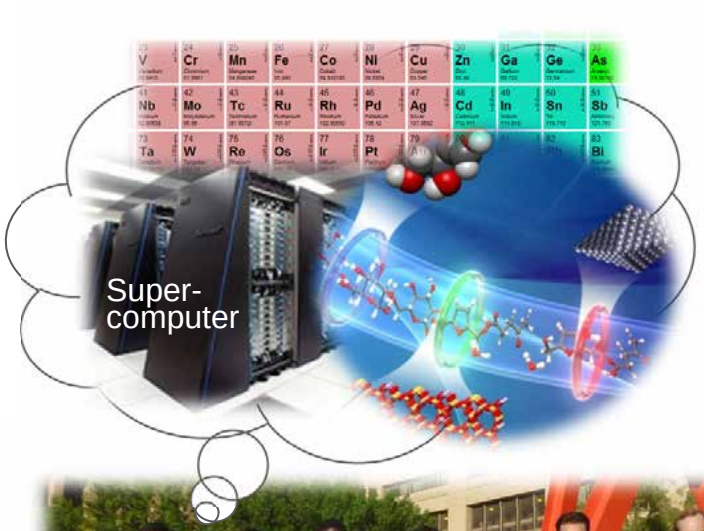
Computational Materials Design and Discovery

Energy and Electronic Applications

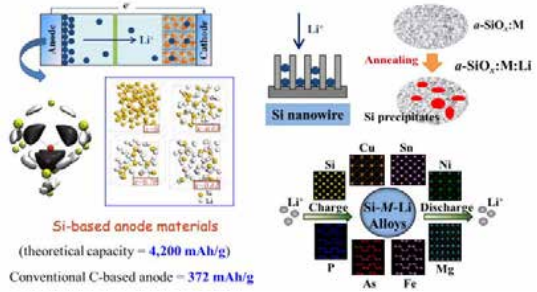
Synthesis → Structure → Properties

Supercapacitors

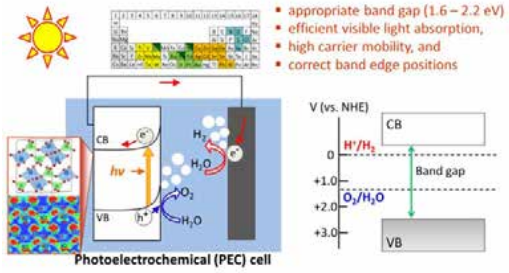




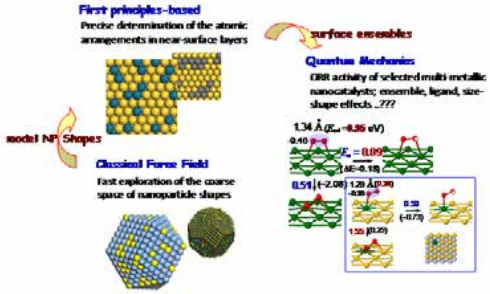
Rechargeable batteries



Photocatalysts

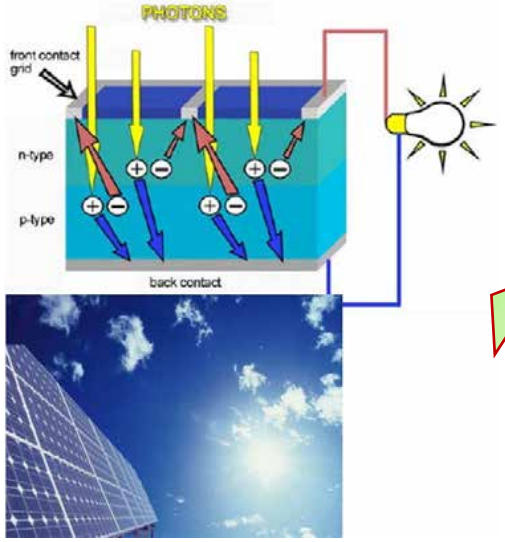


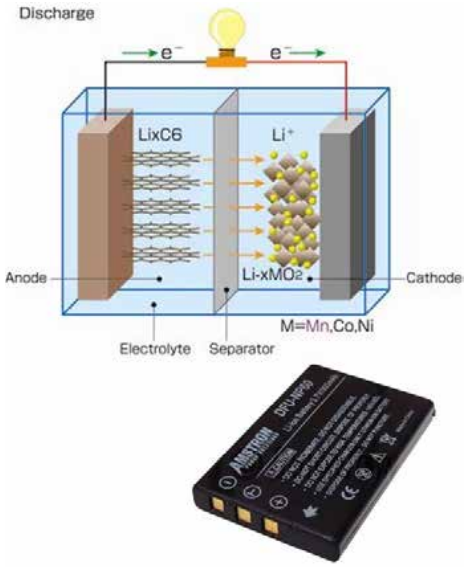
Fuel cell catalysts

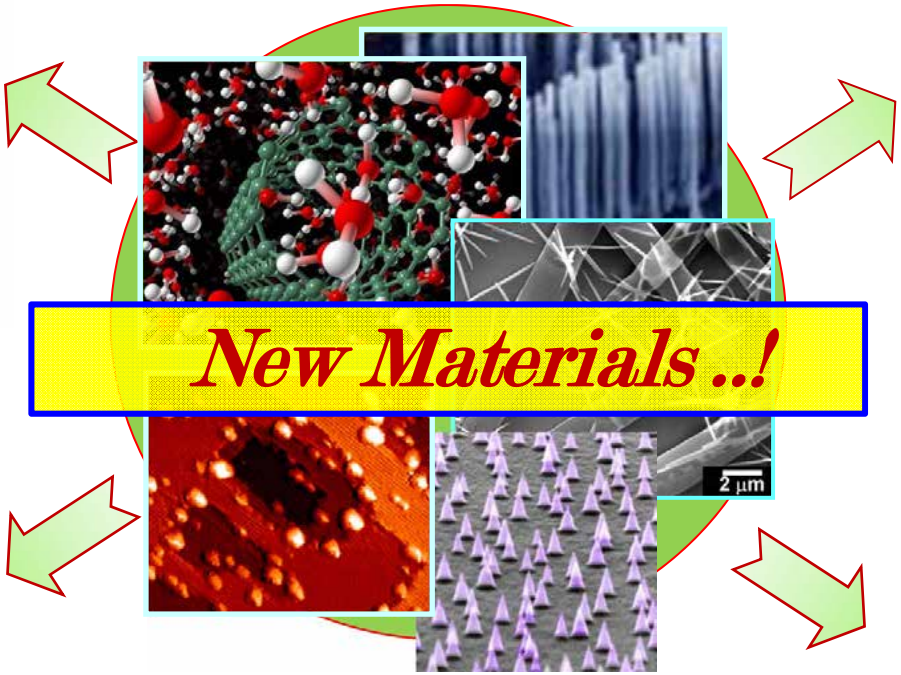


First principles-based computations can provide invaluable guidance on the rational design and synthesis of new materials with desired properties, without slow and costly try-and-modify test and manufacturing cycles!

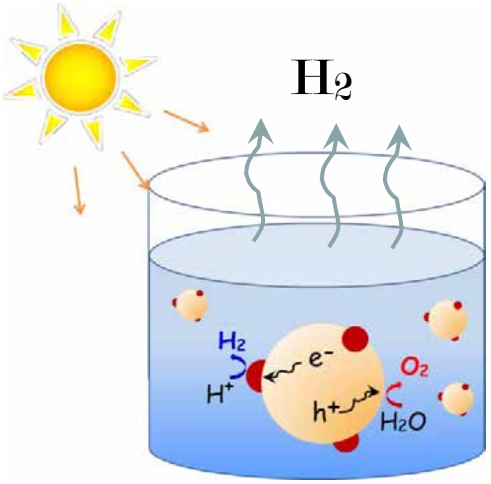
Materials Challenges

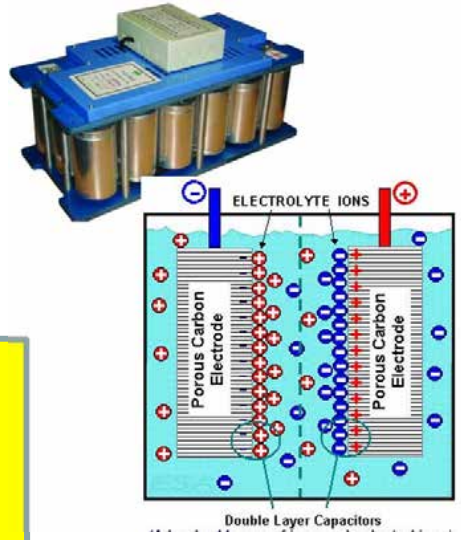






New Materials ..!



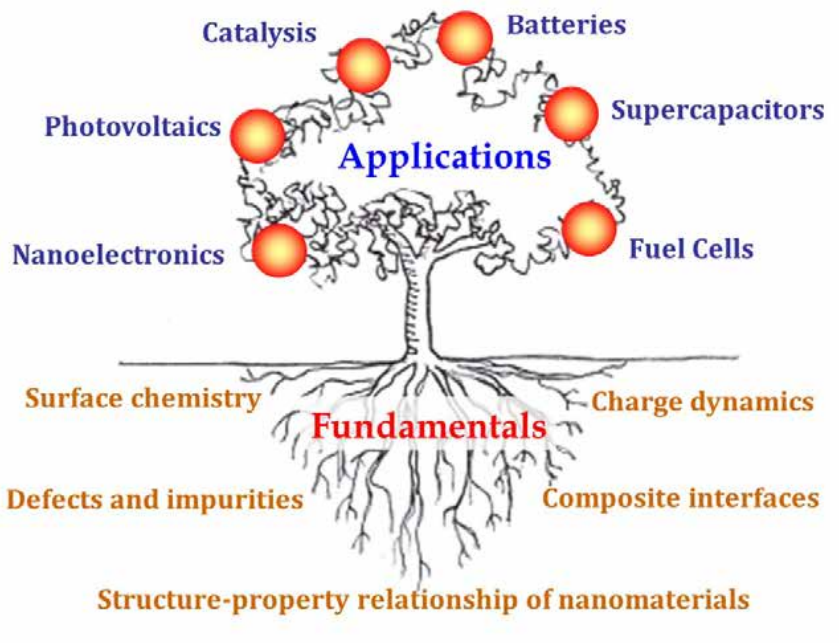


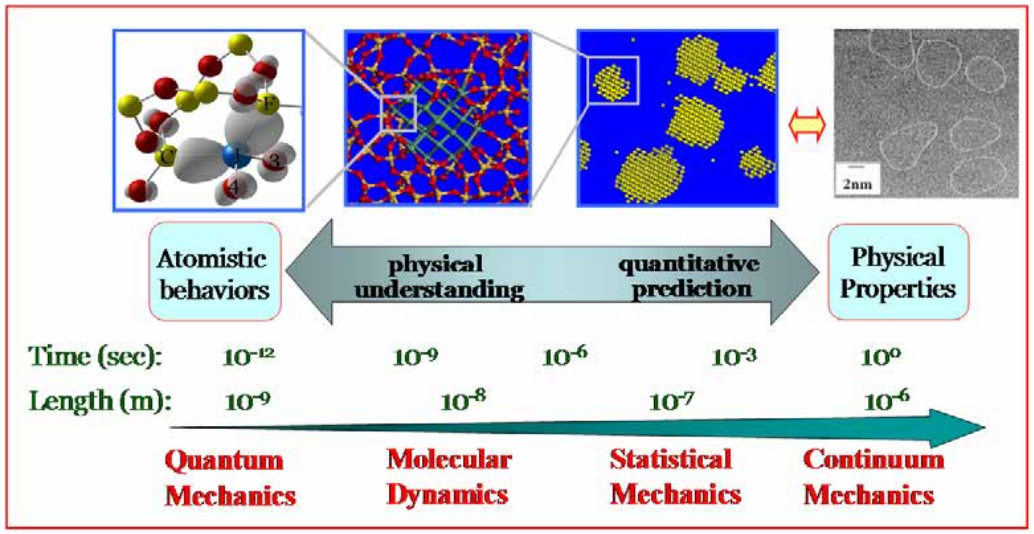
- **Cheap**
- **Abundant**
- **Efficient**
- **Safe**

Hwang Research Group

Computational Design of Nanomaterials for Energy and Electronic Applications

Our research has a well-balanced emphasis on





- strategies for predictive multiscale, multiphysics computational models by integrating various state-of-the-art theoretical methods at different length and time scales.
- a quantitative understanding of the relationship between the synthesis, structure, and properties of nanostructured materials and systems.

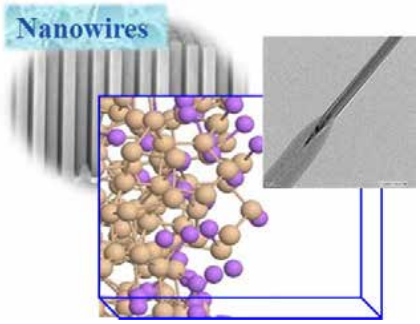
Lithium Ion Batteries

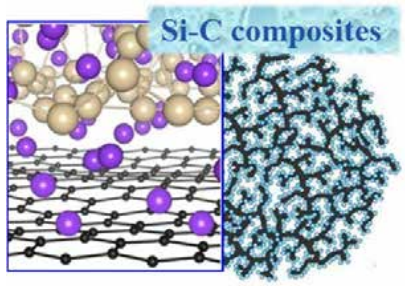
Recent achievements

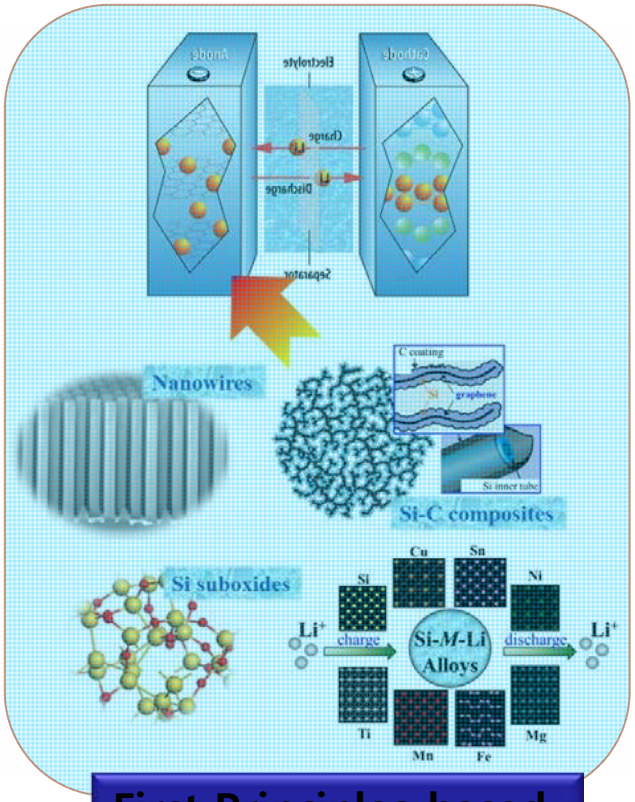
- Elucidate the lithiation mechanisms of silicon-based nanomaterials.
- Provide many insights into how to design nanostructures and composites to achieve desired properties and performance.

Surface/Interface Impacts

- Fast Li diffusion (fast charge rate)
- Facile atomic rearrangement & Uniform lithiation/delithiation (improved cyclability)



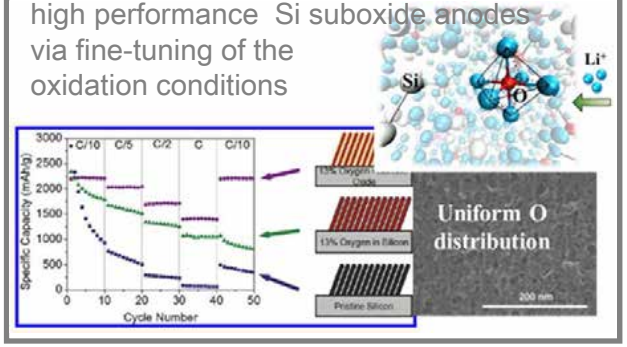




First Principles-based Molecular Modeling

Si-rich suboxides

… highlights the possibility of designing high performance Si suboxide anodes via fine-tuning of the oxidation conditions



Recent Publications

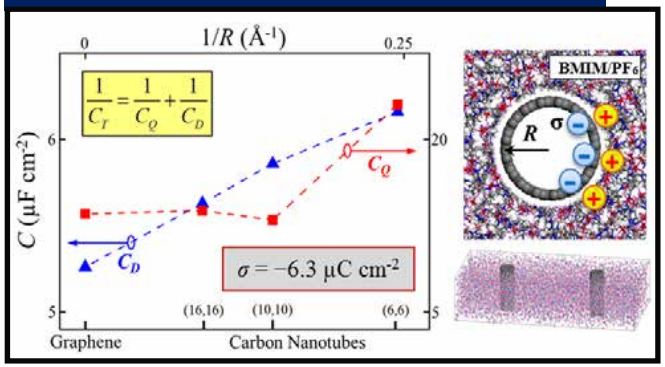
1. Appl. Surf. Sci. 323, 78 (2014)-invited
2. J. Power Sources 263 C, 252 (2014)
3. Chem. Mater. 25, 3435 (2013)
4. J. Phys. Chem. C 117, 9598 (2013)
5. Surf. Sci. 612, 16 (2013)
6. J. Phys. Chem. C 115, 20018 (2011)
7. J. Phys. Chem. C 115, 2514 (2011)
8. J. Phys. Chem. C 114, 17942 (2010)

Graphene-based Supercapacitors

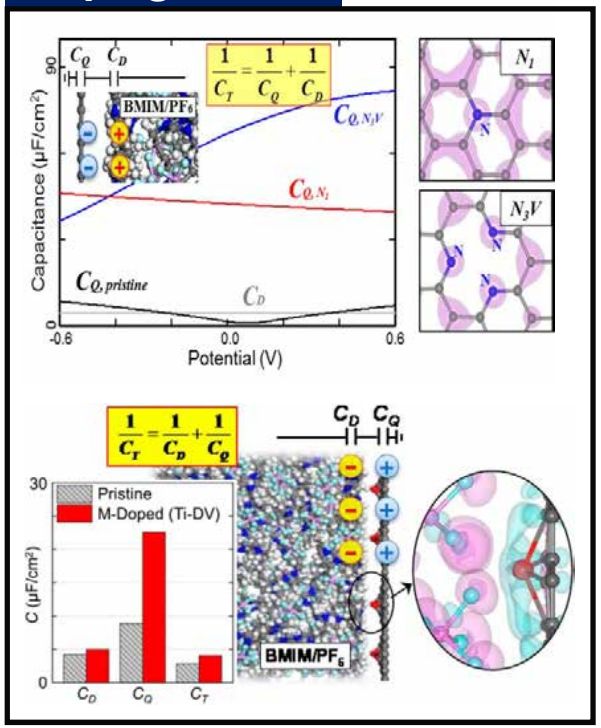
Recent achievements

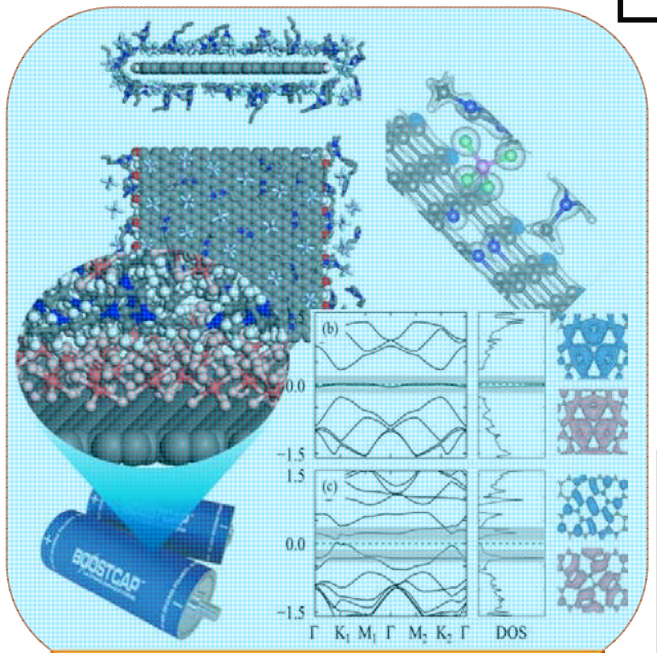
- Identify the key factors determining the interfacial capacitance of graphene-based supercapacitors
- Provide new insight into the impacts of the chemical and/or mechanical modifications of graphene-like carbon electrodes on the supercapacitor performance.

Structural deformation effect

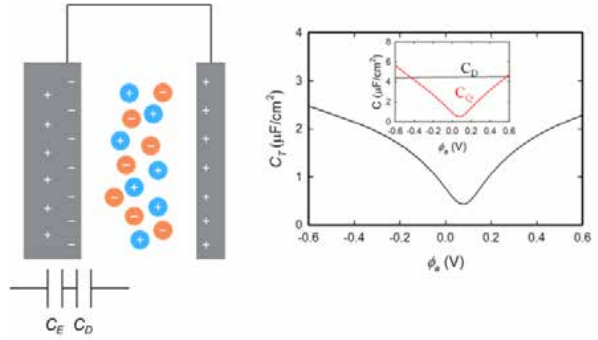


Doping effect





First Principles Modeling



Recent Publications

1. J. Chem. Phys., accepted (2014)
2. J. Phys. Chem. C 118, 21770 (2014)
3. ACS Appl. Mater. Interfaces 6, 12168
4. Carbon 68, 734 (2014)
5. J. Phys. Chem. C 117, 23539 (2013)
6. Phys. Chem. Chem. Phys. 15, 19741
7. J. Phys. Chem. C 117, 5610 (2013)
8. J. Electrochem. Soc. 160, A1 (2013)

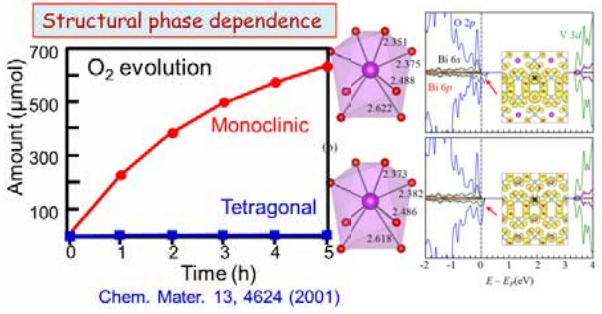
Solar-powered H_2 Production

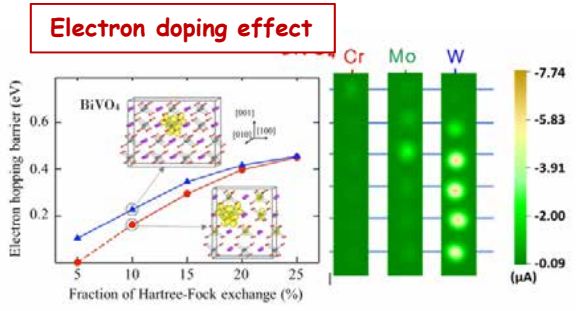
Recent achievements

- Elucidate the effects of chemical doping and structural distortions on charge carrier localization and transport, and their impacts on the photocatalytic performance.
- Identify the role of photogenerated charge carriers in promoting surface reactions.

Doping/Structural distortion

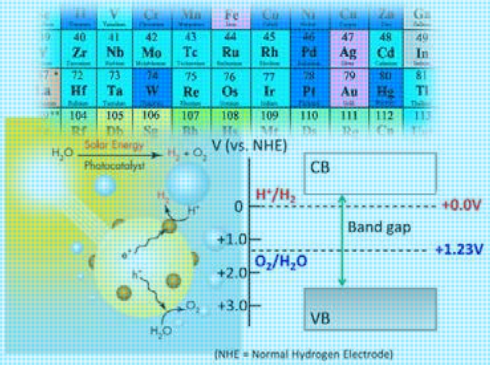
- Band gaps and band alignments
- Charge localization and transport
- Defect formation and properties





Computational Screening, Design & Evaluation

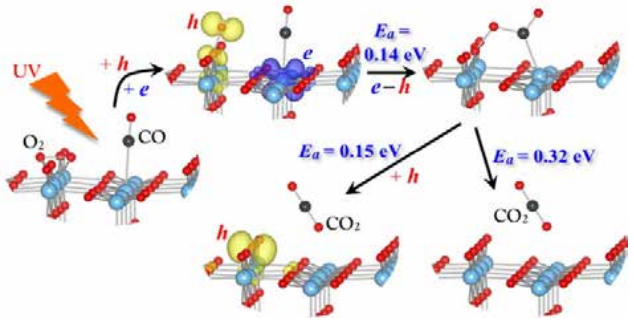
Candidate Photocatalysts



- Visible light absorption (Band gap = 1.6-2.2 eV)
- Correct band edge positions
- High charge carrier mobility
- Low defect density
- High surface reactivity
- High resistance to photocorrsion

Photocatalytic reaction

… highlights that excess electrons and holes can synergetically contribute to CO photooxidation on TiO_2(110) under UV irradiation.



Recent Publications

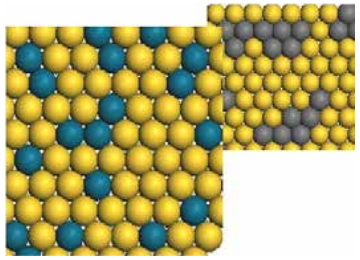
1. ACS Catal. 4, 4051 (2014)
2. Phys. Chem. Chem. Phys. 17, 256 (2015)
3. Appl. Phys. Lett. 103, 131603 (2013)
4. Phys. Rev. B 87, 205202 (2013)
5. Phys. Rev. B 86, 165209 (2012)
6. J. Phys. Chem. C 115, 17870 (2011)
7. More coming soon …

Electrocatalysis in Fuel Cells

Develop low-Pt or Pt-free metal catalysts that are more active, more abundant, and less expensive than the currently used Pt-based catalysts.

First principles-based

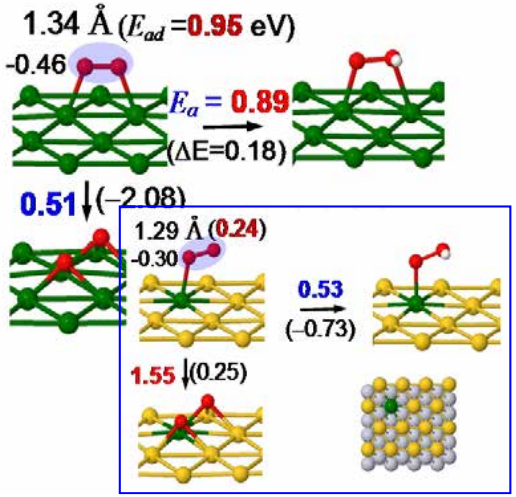
Precise determination of the atomic arrangements in near-surface layers



surface ensembles

Quantum Mechanics

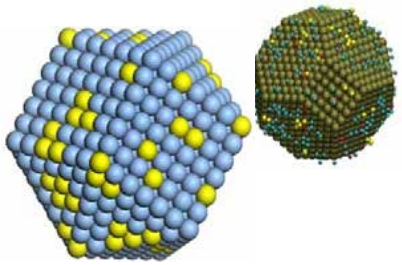
ORR activity of selected multimetallic nanocatalysts; ensemble, ligand, size-shape effects ..???



model NP Shapes

Classical Force Field

Fast exploration of the coarse space of nanoparticle shapes



Recent Publications

1. J. Chem. Phys. 139, 201104 (2013)
2. Chem. Soc. Rev. 42, 5002 (2013)
3. J. Am. Chem. Soc. 135, 436 (2013)
4. Phys. Chem. Chem. Phys. 15, 12118
5. J. Chem. Phys. 139, 164703 (2013)
6. Chem. Mater. 25, 530 (2013)
7. J. Phys. Chem. Lett. 3, 566 (2012)
8. J. Phys. Chem. C 115, 21205 (2012)
9. Catalysis Today 165, 138 (2011)
10. J. Phys. Chem. C 114, 21516 (2010)
11. J. Phys. Chem. C 114, 14922 (2010)
12. J. Phys. Chem. C 113, 12943 (2009)

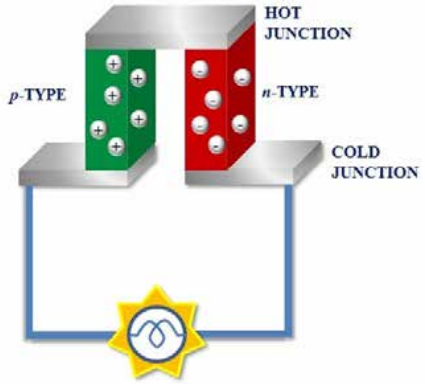
Multiscale Modeling Strategy for screening multimetallic electrocatalysts

Waste Heat Conversion into Electricity

Understand the properties and performance of nanomaterials for thermoelectric applications with a particular focus on their thermal conductivity

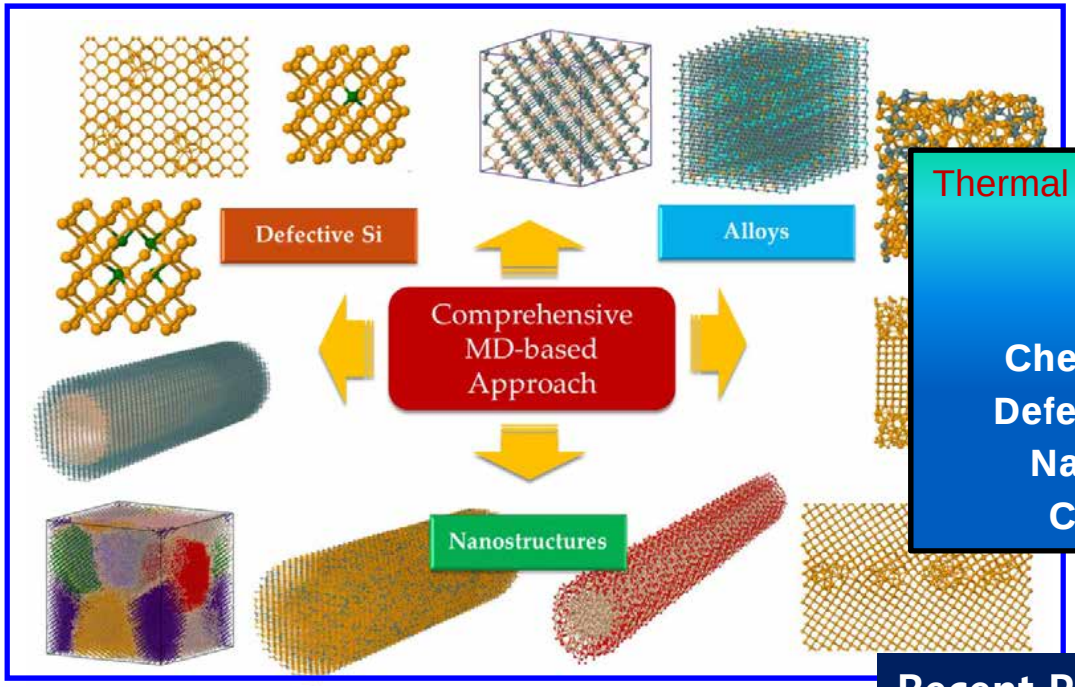
Heat ↔ Electricity

$$ZT = S^2 \sigma T / \kappa$$



Seebeck Effect

Temperature gradient ↕ Electricity



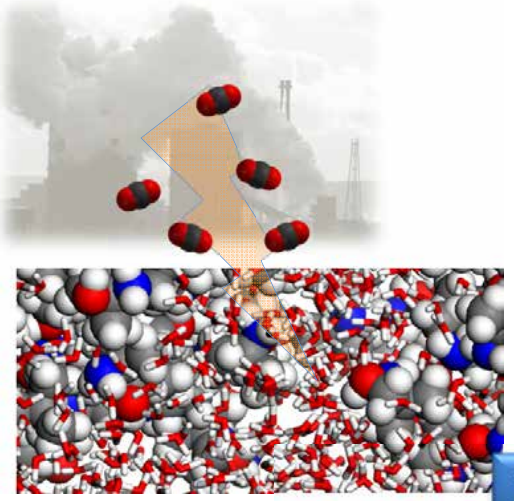
Thermal Conductivity Control via

Alloying
Chemical Doping
Defect engineering
Nanostructuring
Compositing

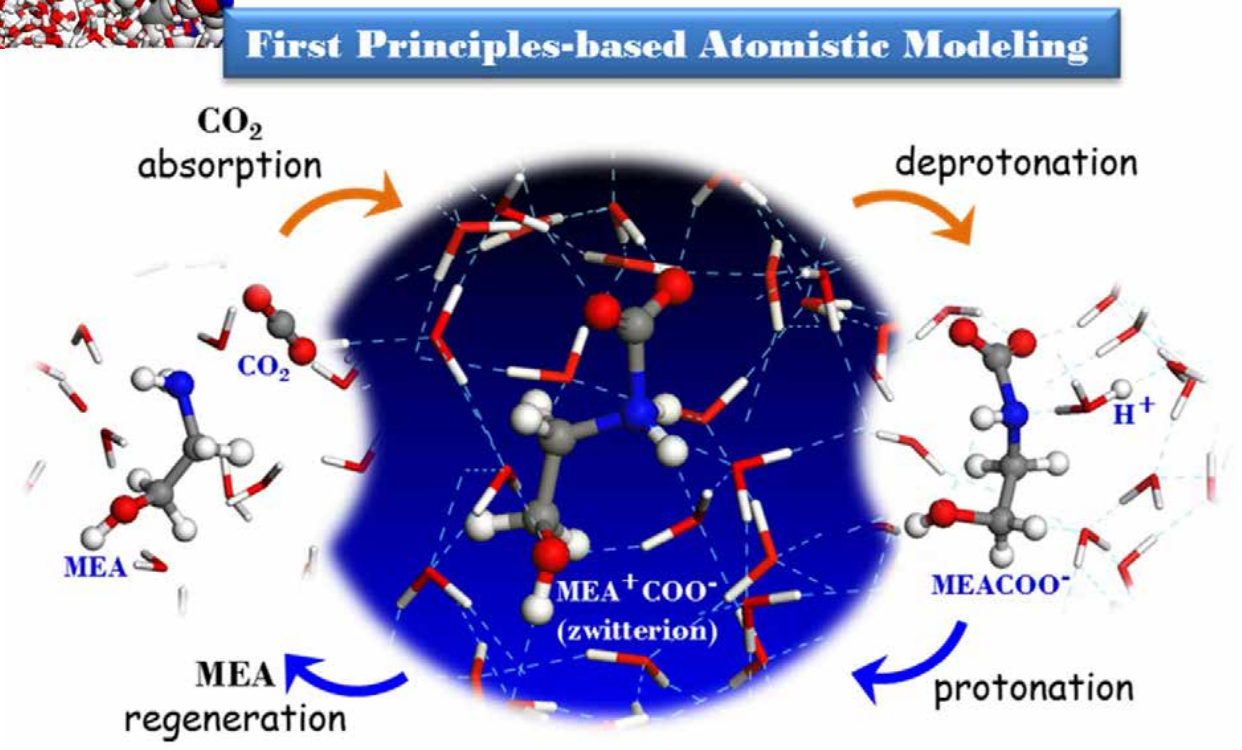
Recent Publications

1. J. Appl. Phys. 114, 174910 (2013)
2. Phys. Rev. B 86, 165209 (2012)
3. Nano Lett. 12, 2918 (2012)
4. Phys. Rev. B 85, 125204 (2012)
5. Phys. Rev. B 83, 125202 (2011)
6. More coming soon

CO_2 Capture and Conversion



.... provide the guiding principles for the rational design and synthesis of novel regenerable amine-based solvents to realize the desired properties and performance for CO_2 capture, through systematic theoretical investigations of the atomistic mechanisms governing CO_2 capture and solvent regeneration.



Top-notch Computational Resources

High Performance Computing Systems at UT-Austin (http://www.tacc.utexas.edu)

(1) **"STAMPEDE"**

One of the largest computing systems in the world for open science research.

- 102,400 Processing Cores
- 205 TB Memory
- 7+ Petaflops of Peak Performance

(2) **"LONESTAR"**

One of the most powerful academic supercomputers in the world.

- 22,656 Processing Cores
- 44 TB Memory
- 300+ Teraflops of Peak Performance

Successful completion of our extensive first principles-based investigations can be facilitated by utilizing the world's top-class supercomputing facilities.