Massachusetts Institute of Technology

G^{2}e
Grossman Group of Clean Energy

Computing Requirements for

Computational Design of Novel Energy Materials

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NERSC BES Requirements for 2017
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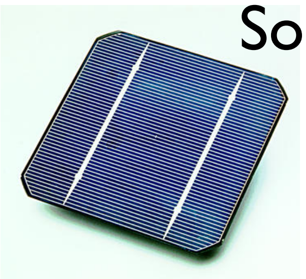
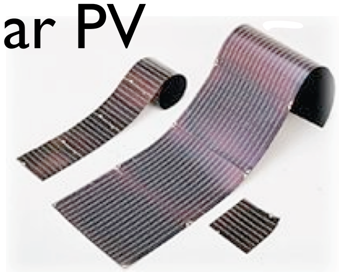
Materials will shape the future of renewable energy

Solar PV

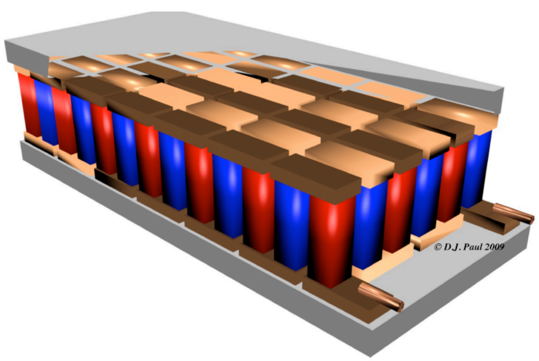


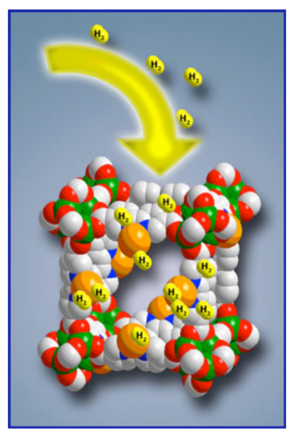


Biofuels

Batteries

Thermoelectrics

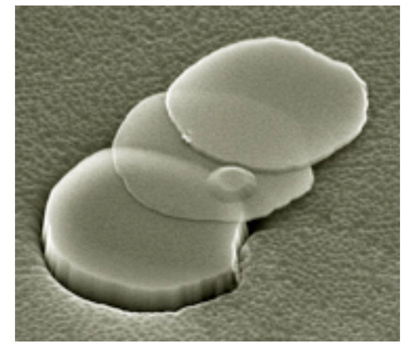


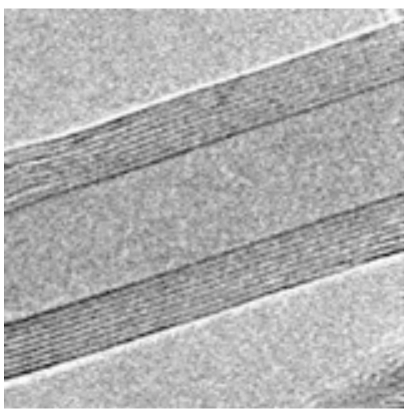


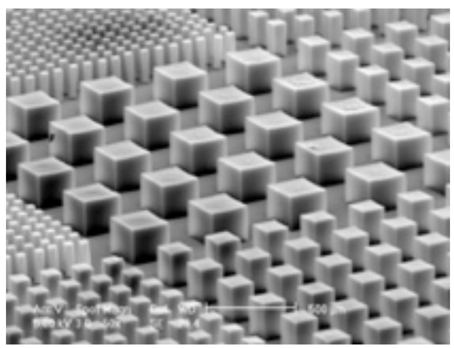
Hydrogen Storage

Solar Thermal

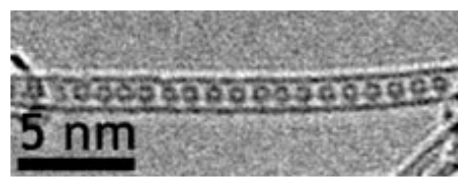
Example of a single element

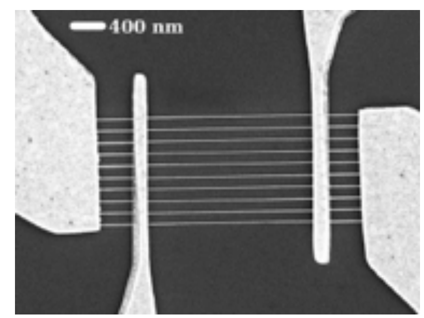






Carbon





Carbon in energy to date

One Barrel of oil =
1.73 MWh of energy

Burning Carbon for energy

Same carbon, different use

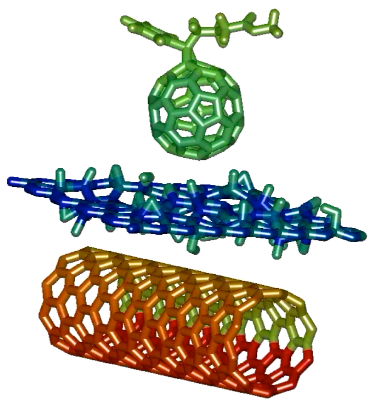
Using 1% of carbon in the same 1 barrel to make plastic for thin-film solar cells.

One Barrel of oil =
16,000 MWh energy
(5% efficient, 1 year)

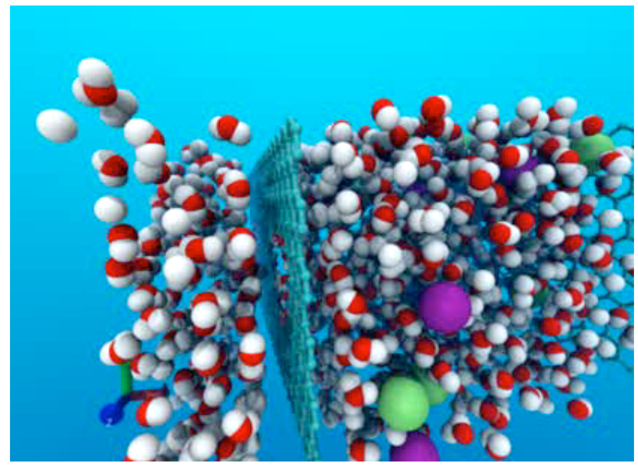
Solar cells

10,000 X more energy from same material!

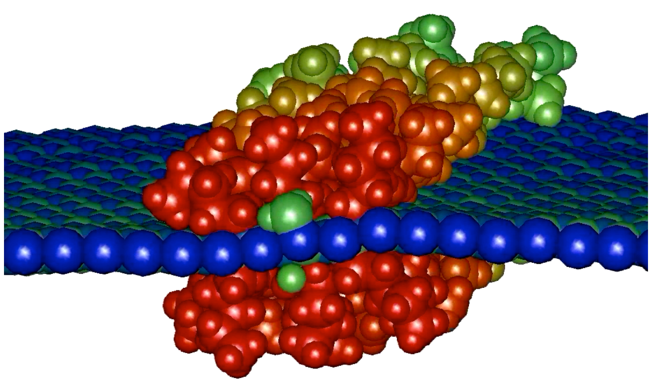
Beyond burning: a carbon materials energy future



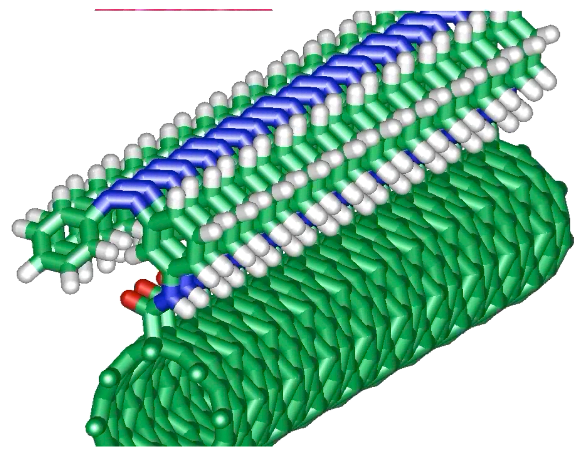
All-Carbon Solar Cells



Water desalination



Thermoelectrics



Solar thermal fuels

Summary of Projects in 2013

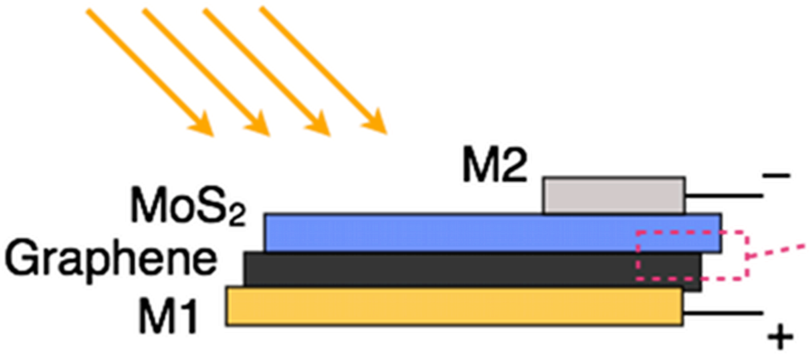
m655, Quantum simulation of nanoscale energy conversion

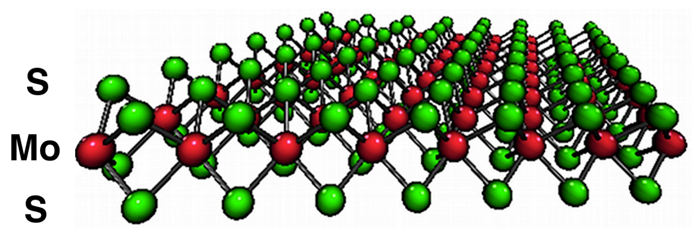
- Solar Cells Based on Monolayer Materials
- Energy alignment in Metal/Organic Interfaces and its effect on solar cell efficiency
- Thermal and electronic transport in patterned graphene for thermal electric applications

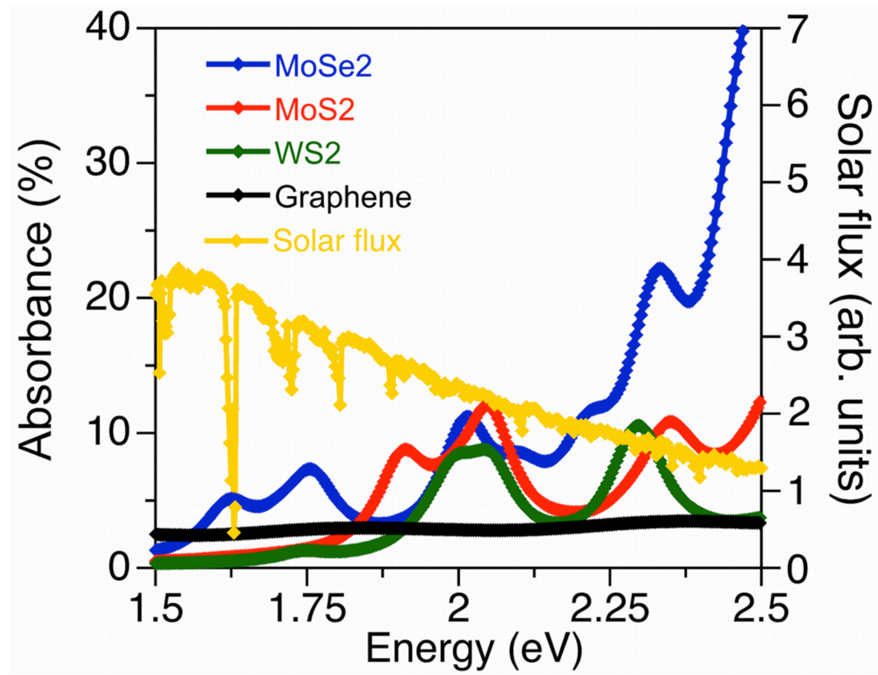
m1797, Design of high-efficiency solar thermal fuels via first-principles computations

- Optical properties and excited state dynamics of STF
- High-throughput search of novel STF materials

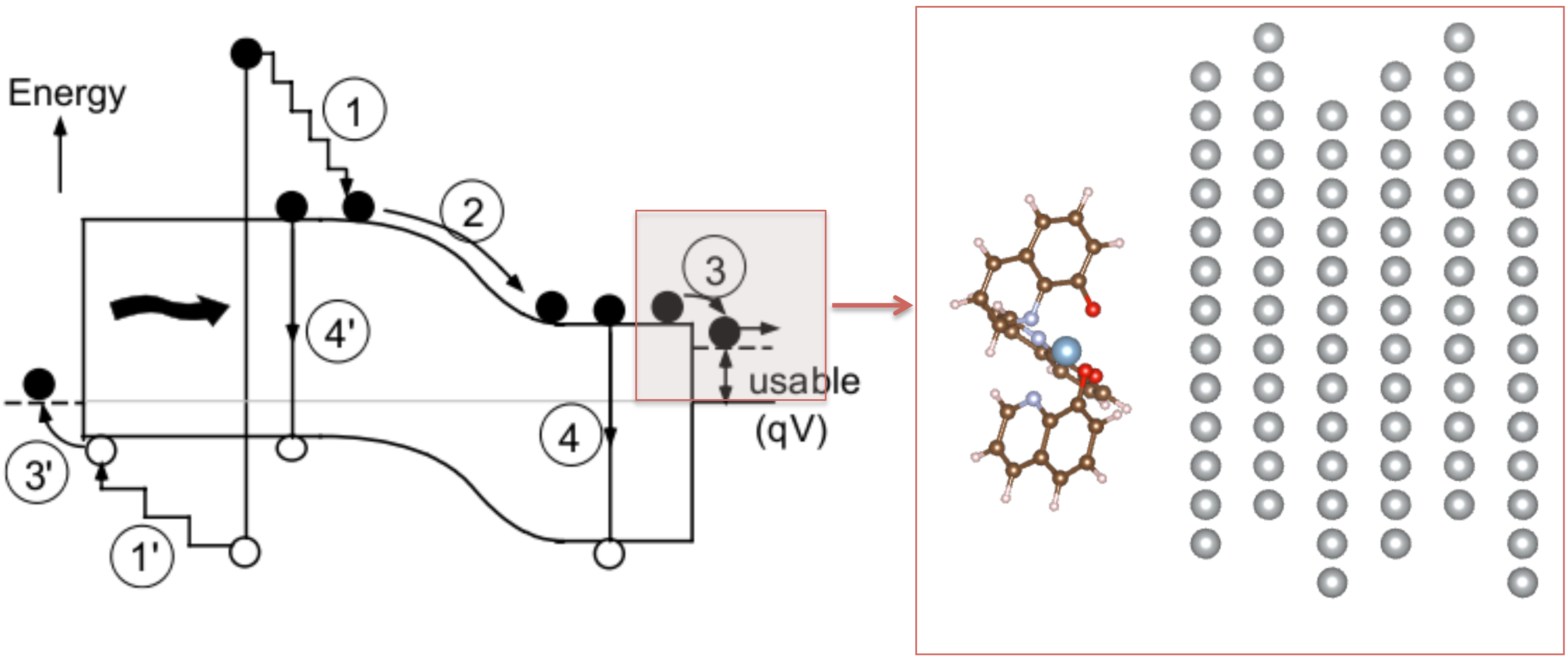
Two-Dimensional Monolayer Materials for Ultra-Thin Excitonic Solar Cells



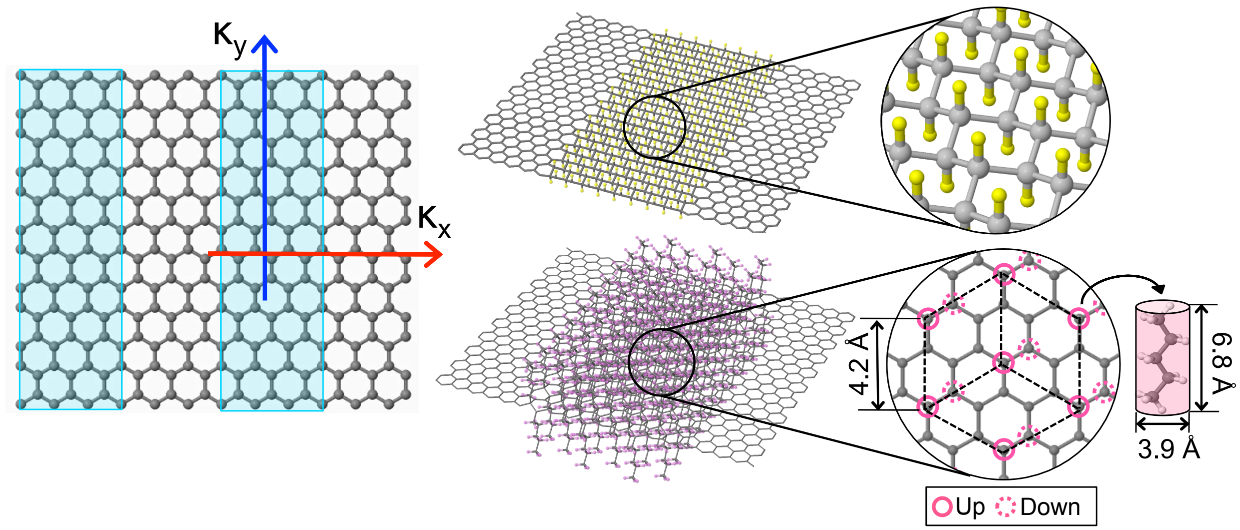




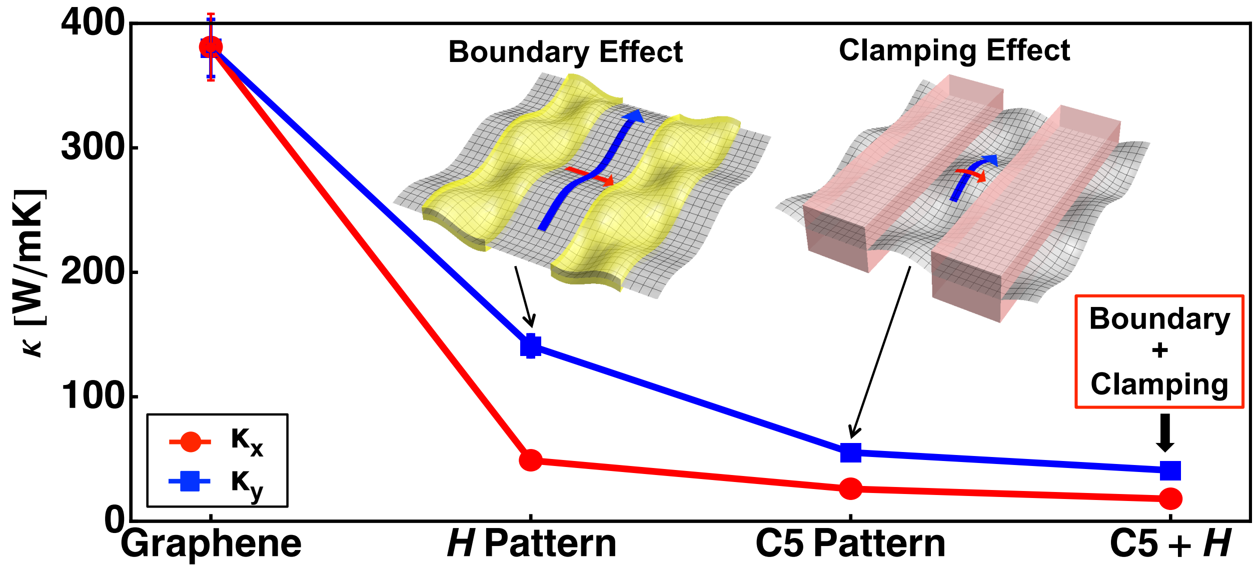
Maximize Energy Efficiency in Solar Cells at Metal-Organic Interfaces



Chemically Functionalized Graphene for Thermoelectric Applications



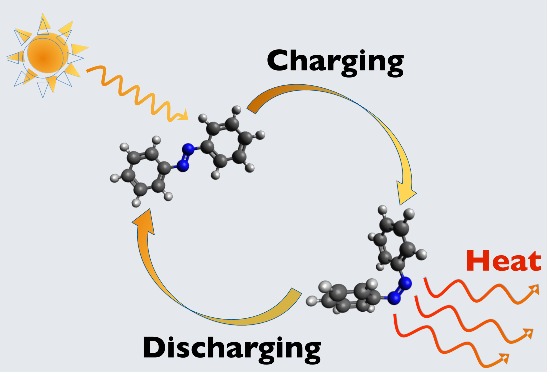
Patterned 2D shapes on graphene reduces the room-temperature thermal conductivity.



Due to a combination of boundary and clamping effects.

High Throughput search of STF materials

Solar Thermal Fuel (STF)



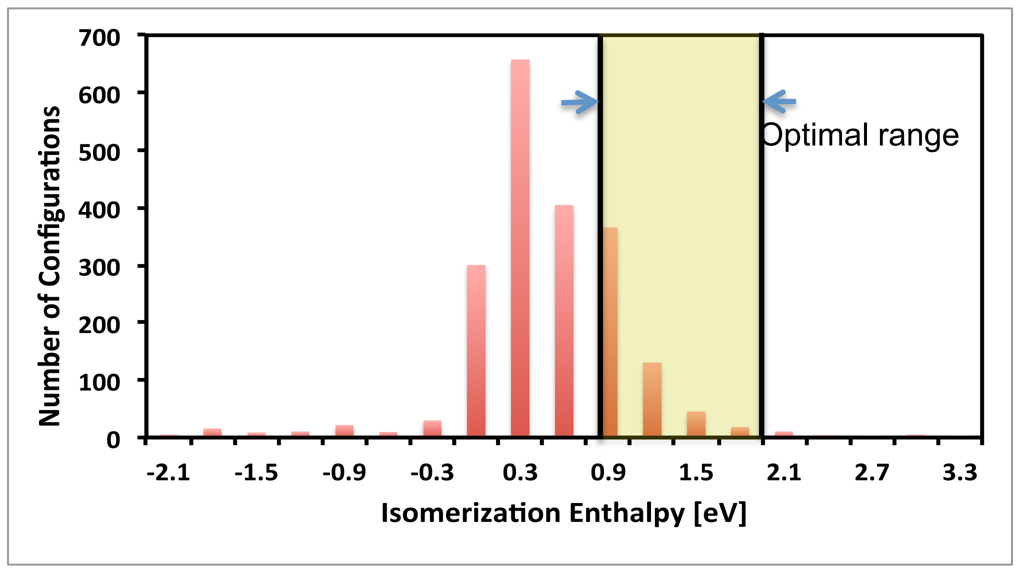
Challenges:

- Increase stability
- Higher energy density
- Lower cost

High Throughput search

Screen through databases of molecules

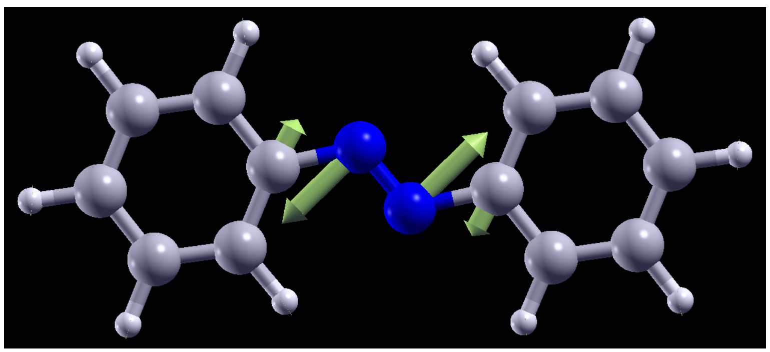
Better STF candidates (2000 discovered)



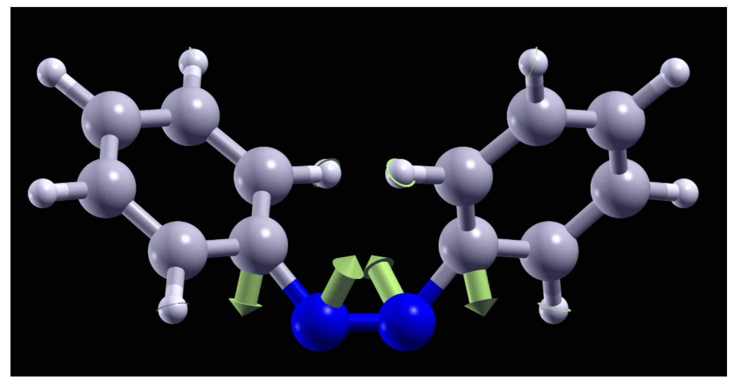
Photoisomerization Dynamics for Solar Thermal Fuels

Excited-state forces in time-dependent density-functional theory

Excited state for trans-azobenzene



Excited state for cis-azobenzene



Access to dynamics of complicated systems (e.g. azobenzene + nanotube)

octopus

Future research topics (by 2017)

- Patterning and functionalization in 2D materials for solar cell.
- Functionalization of patterned graphene for thermal electric applications.
- Photophysics of STF with templates and functionalized groups.
- High-throughput (HT) design of STF materials with newly discovered design principles.

Computational Strategies

- We employed empirical MD, DFT, TDDFT, GW and Bethe-Salpeter equation calculations.
- The codes we use are LAMMPS, VASP, Gaussian, Octopus, Quantum-Espresso, and our own java-based HT code.
- Our biggest computational challenges are from simulations of large patterned structures with functionalization (>500 atoms).
- Our parallel scaling is mostly limited by parallelization efficiency of VASP on more than 2000 cores.
- We expect to use the same (or similar) set of codes by 2017. One of our group member (David Strubbe) is a developer of the Octopus code for TDDFT simulations.

Current HPC Usage

- We have 14M SUs in 2013, mostly running on Hopper
- Typical run on 100~1000 cores for 48 hours, around 2000 jobs a year.
- 2TB data read/written per run
- Typically use 2GB~4GB memory per core, 1.5T aggregate memory per run.
- Besides standard HPC services, we asked for code compilation assistance as well as optimization advice.
- We use 10TB scratch file system, 7TB shared file system and 7TB archival space except for the High Throughput simulations.
    - HT simulation along can generate 10TB scratch file and 5TB data at a time.

HPC Requirements for 2017

- Around 100M SUs needed except HT simulations by 2017.
  - HT simulations along may take 100M SUs, depending on the configuration space explored.

- We expect to run concurrently on 1000~64000 cores for 48 hours per job. 2000 jobs per year.

- Data read/write will increase by a factor of 5 to 10TB as a result of increased system size except HT simulations.
  - HT simulations may generate 1PB scratch and 500TB data at a time.

- Memory per core will increase by a factor of 4 to 8GB/core considering increased parallelization. Aggregate memory usage per run will reach 50TB.

- We would like to ask for code compilation, database server support, web server host service from NERSC.

Summary

- With the expected improvements with NERSC, we will be able to design new energy materials which are currently beyond the simulation power.
- Our researches will be more CPU intensive than I/O intensive, with the exception of disk space. Therefore faster/more CPUs will best benefit our researches.
- With access to 32X your current NERSC allocation, we will for the first time be able to explore a full subset of configuration space with computational materials design.
- Result libraries generated from HT simulations would be of interest to the general materials research community, therefore additional webserver service will become useful by 2017.

Group and Support

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