High-Throughput Computational Materials Design for Catalysis and Renewable Energies

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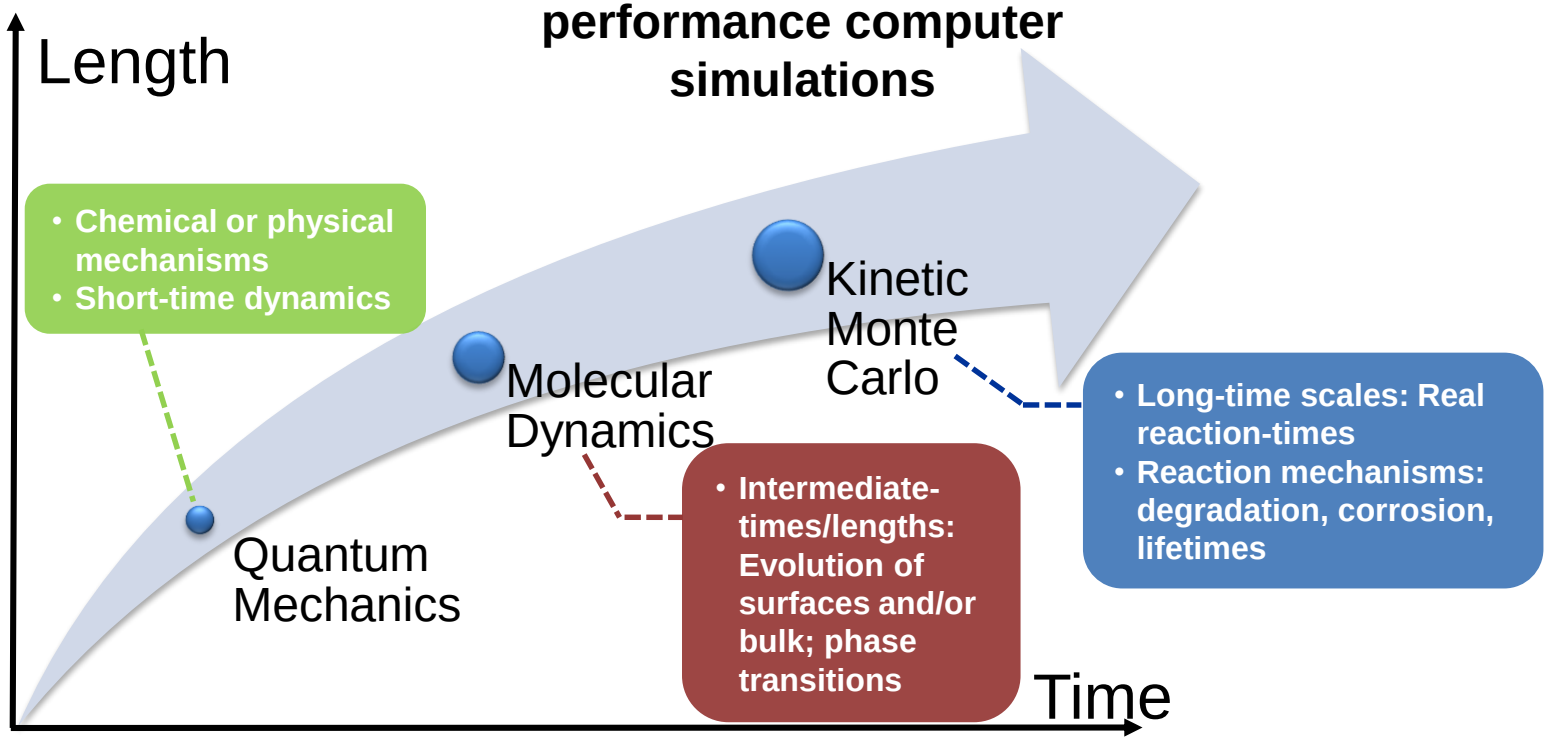
High-Throughput Computational Materials Design

Goals: Understand/predict reaction & degradation mechanisms and dynamic evolution of materials under reaction and/or harsh environmental conditions

Accomplished through high-performance computer simulations



Ada Cluster

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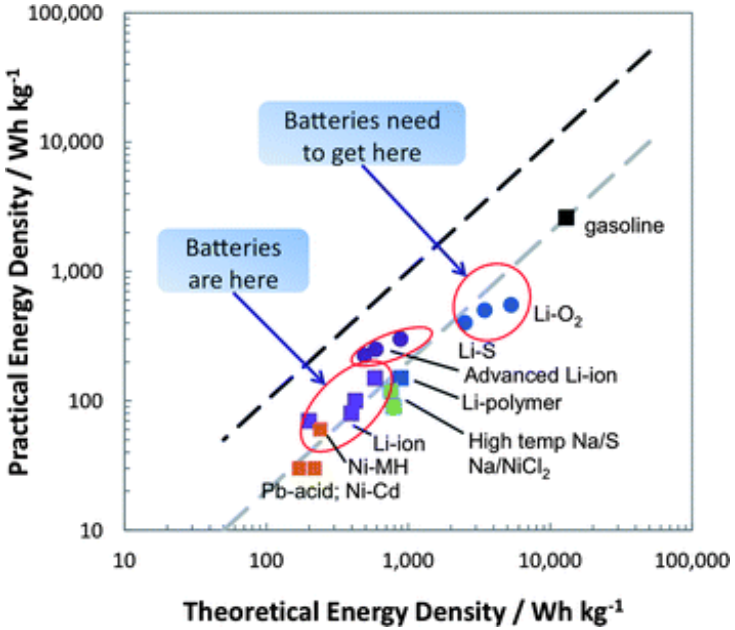
Renewable energies (solar, wind) are intermittent

materials research crucial to develop electric vehicle applications



Batteries store chemical energy

molecular level understanding is vital

Thackeray et al., Energy Environ. Sci., 5, 7854, (2012)

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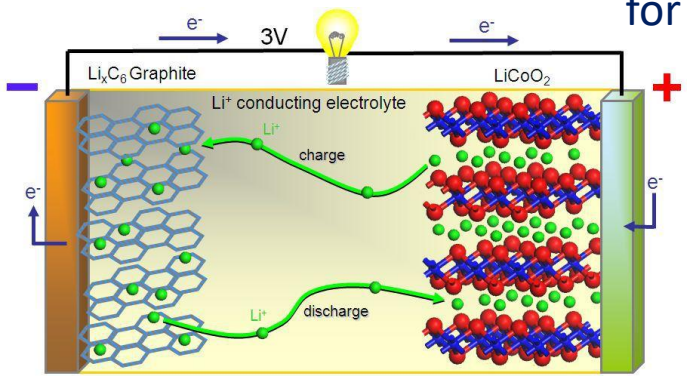
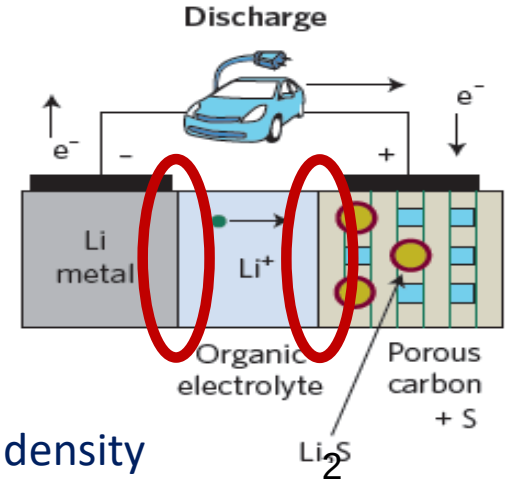
Lithium-ion

for small devices

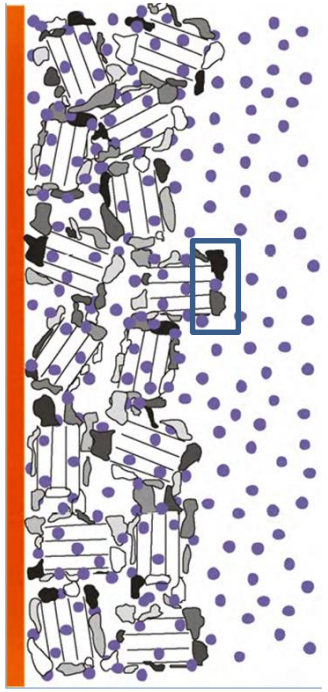


Lithium-Sulfur

for electric cars



higher energy density
but complex chemistry



interfacial reactions generate a multicomponent solid-electrolyte interphase (SEI) film. Its properties are key for the battery lifetime

New insights obtained through DFT and AIMD simulations in high performance computers!!!

software: Gaussian 09, VASP;
hardware: ADA

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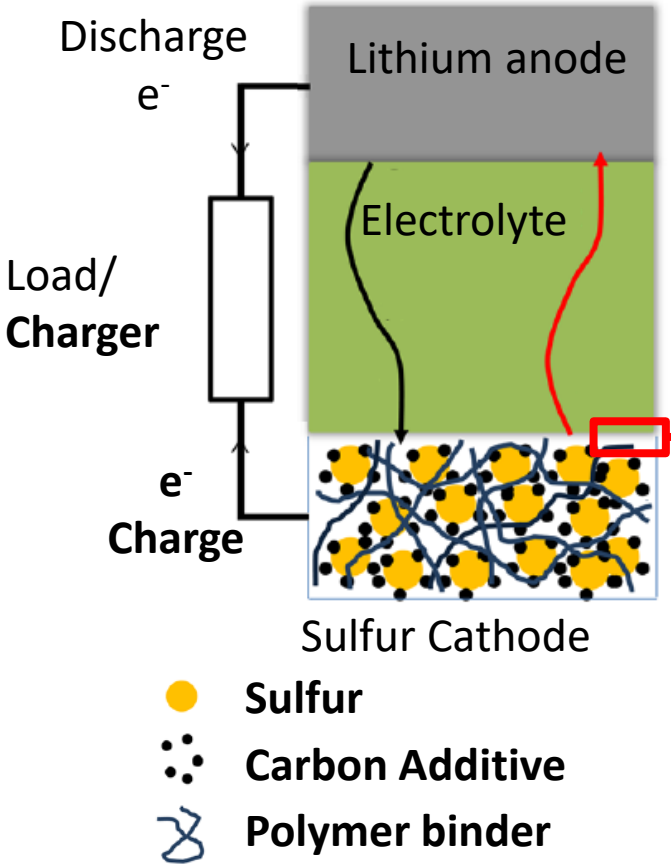
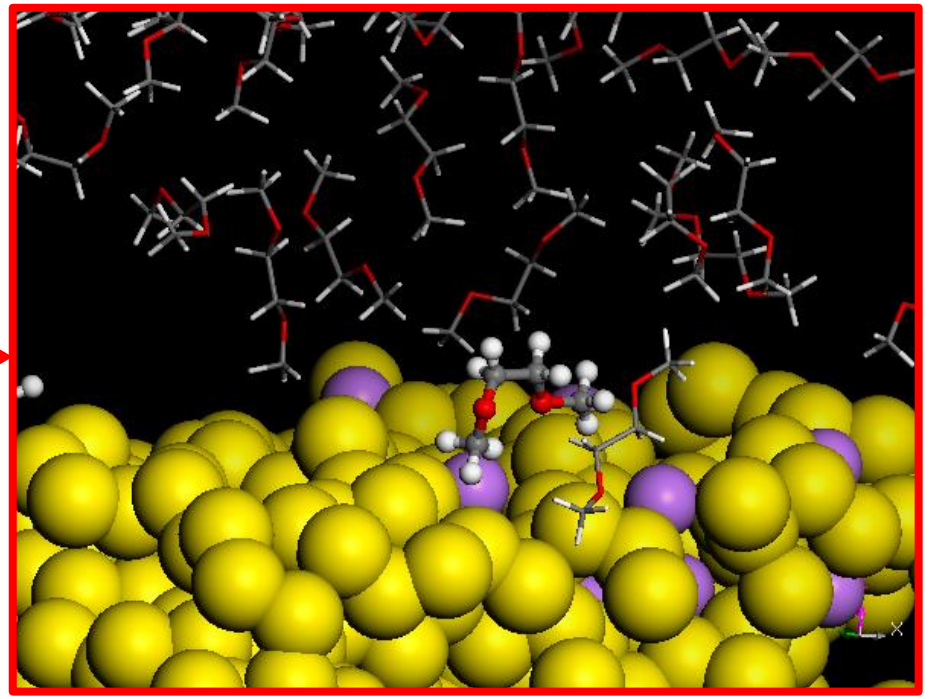
Li-S batteries: Elucidation of the Cathode-Electrolyte Interfacial Chemistry



Theoretical MD/DFT calculations using LAMMPS/VASP



HPC Ada cluster at Texas A&M (IBM NeXtScale Cluster)

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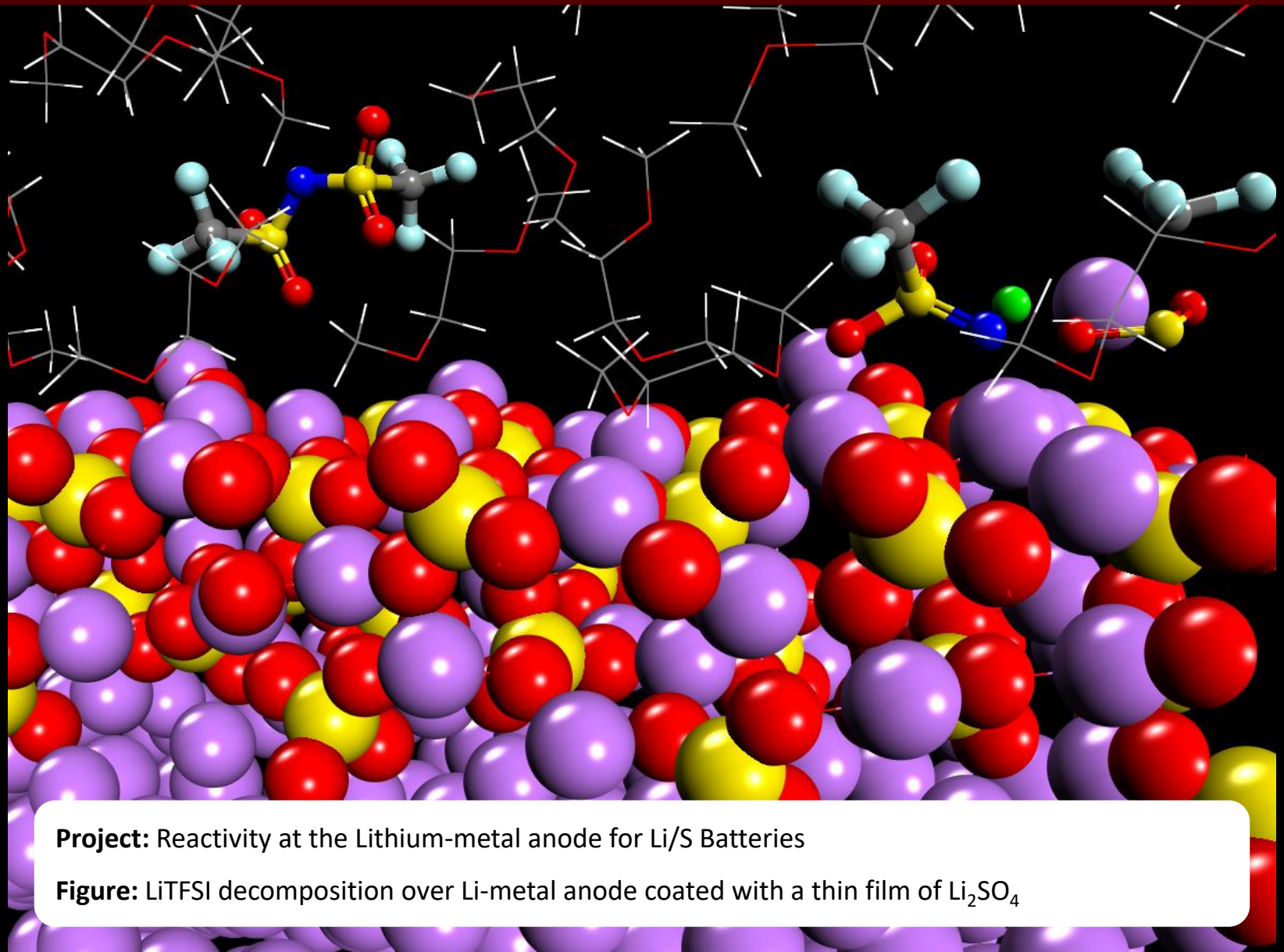

Project: Reactivity at the Lithium-metal anode for Li/S Batteries

Figure: LiTFSI decomposition over Li-metal anode coated with a thin film of Li_2SO_4

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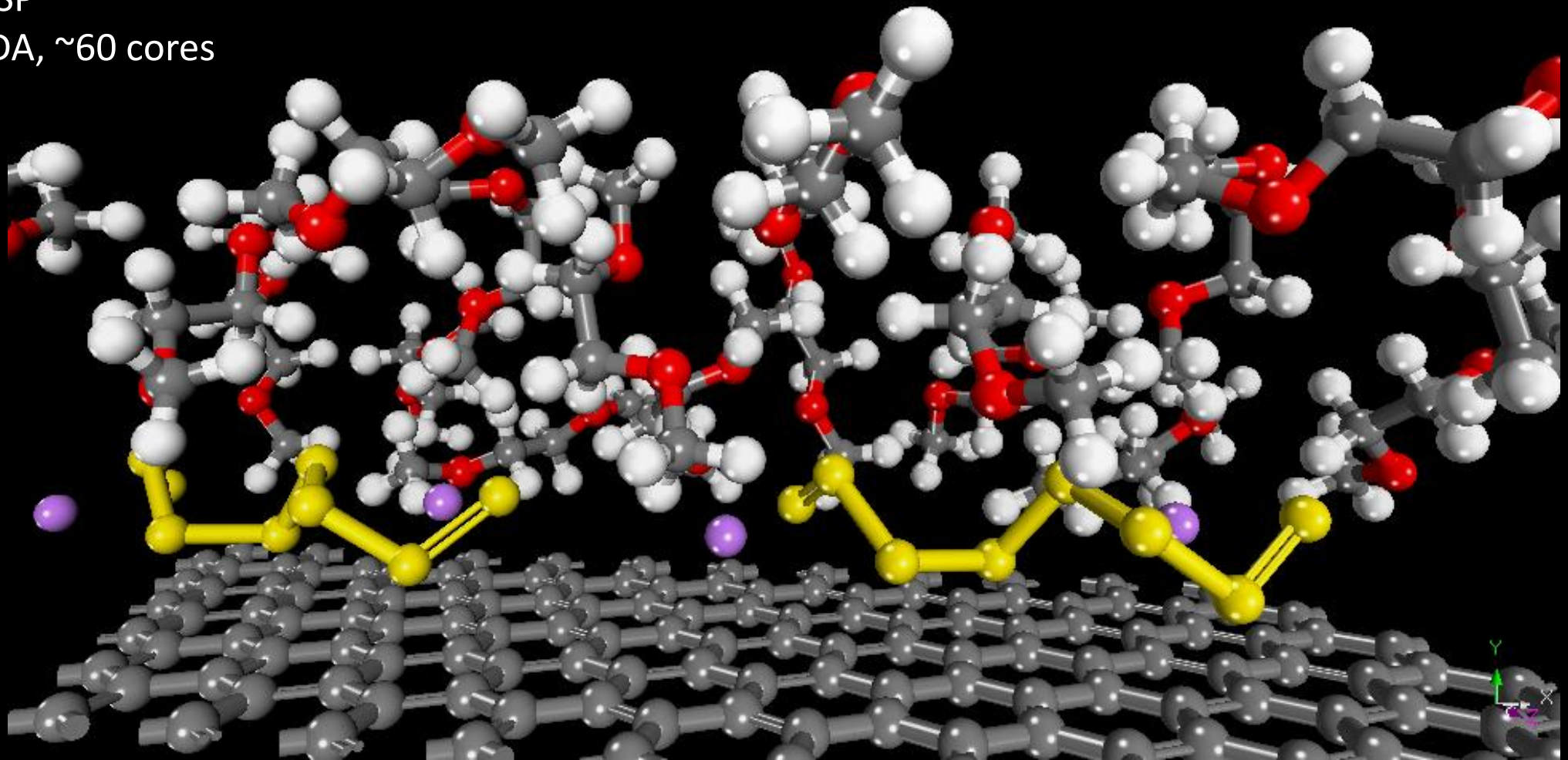
Project: Lithium Sulfur Battery: cathode and electrolyte stability and behavior

Figure: Mixture of DME and polysulfide molecules on top of graphene layer

software: VASP
hardware: ADA, ~60 cores



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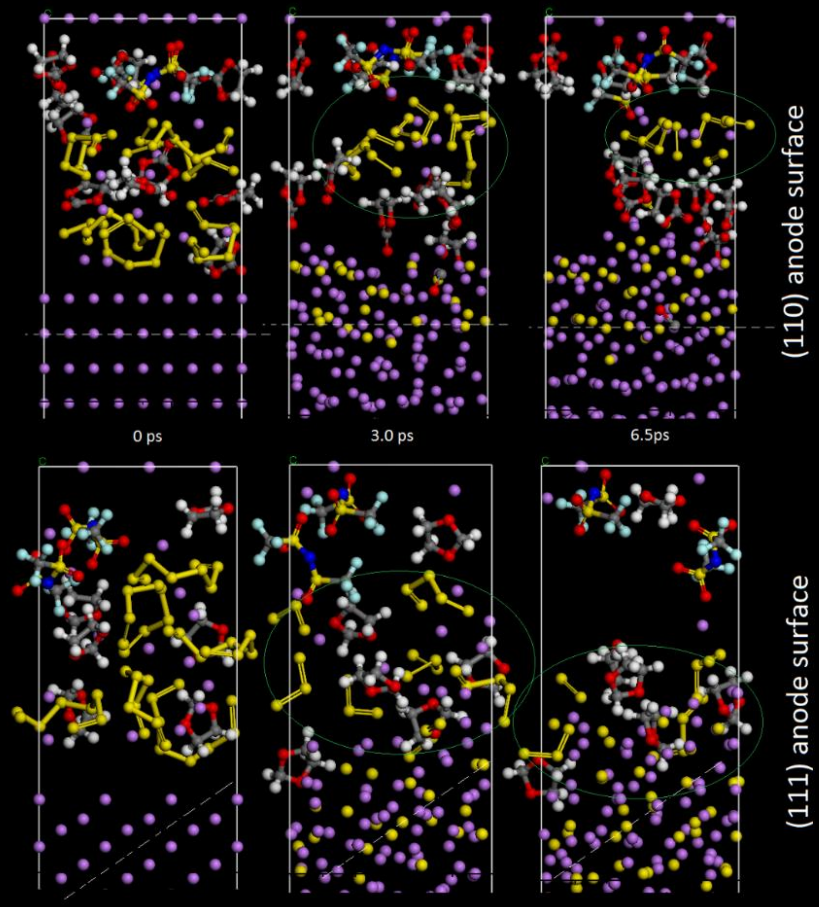
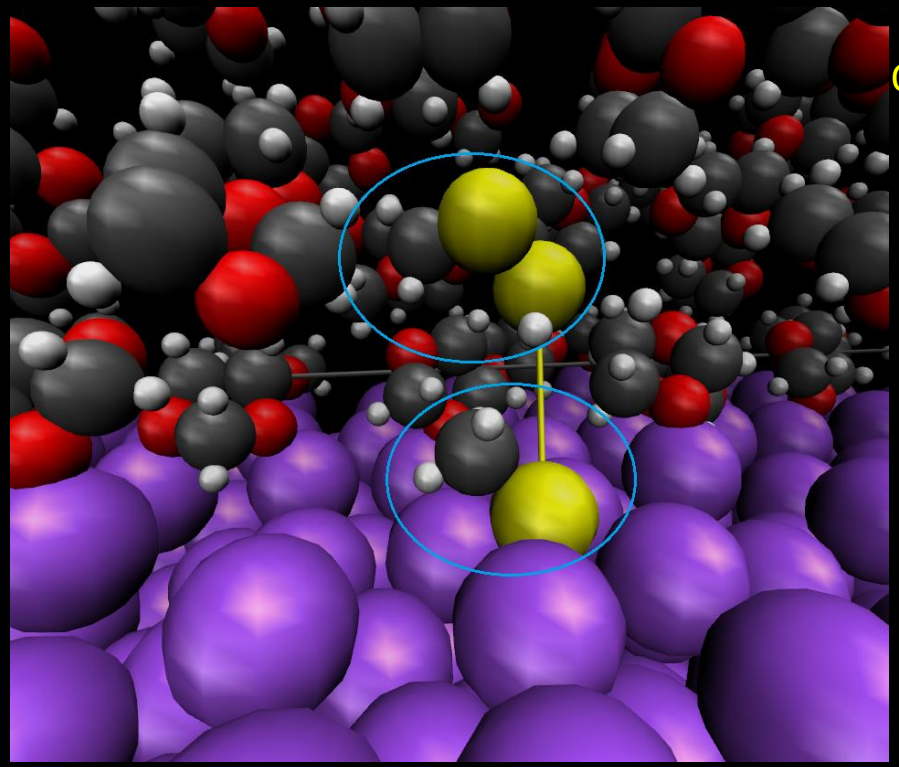
Reactivity of PS and OS on Lithium Anode Surface of Li-S batteries



Reactivity of polysulfide (PS) decomposition on Li metal



Organosulfide (OS) radicals formed at the Li metal surface

DFT-based Studies of the impact of "Shuttle-Effect" on SEI formation

- Oxygen
- Lithium
- Sulfur

software: VASP
hardware: ADA, ~60 cores

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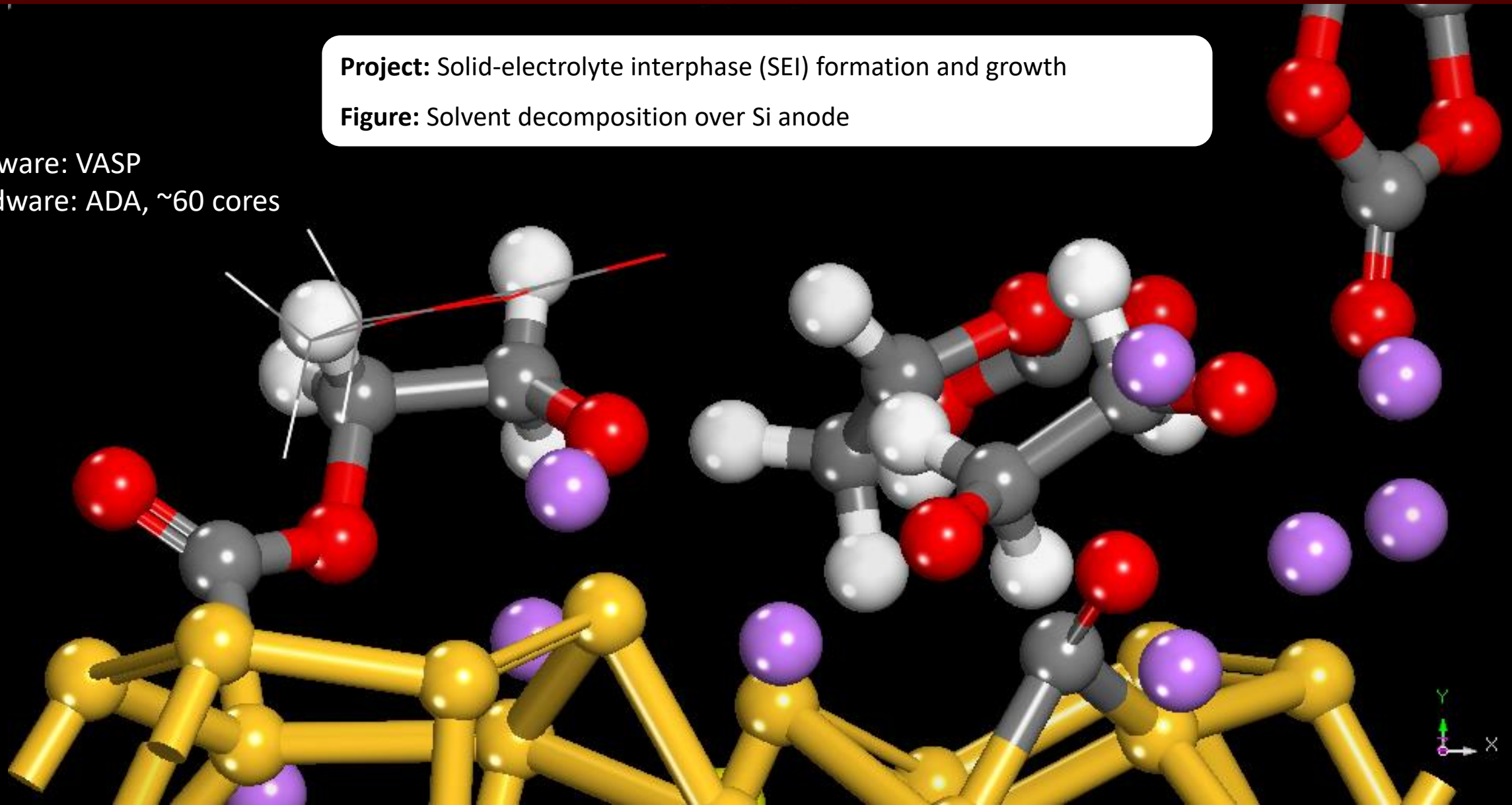
Project: Solid-electrolyte interphase (SEI) formation and growth

Figure: Solvent decomposition over Si anode

software: VASP
hardware: ADA, ~60 cores



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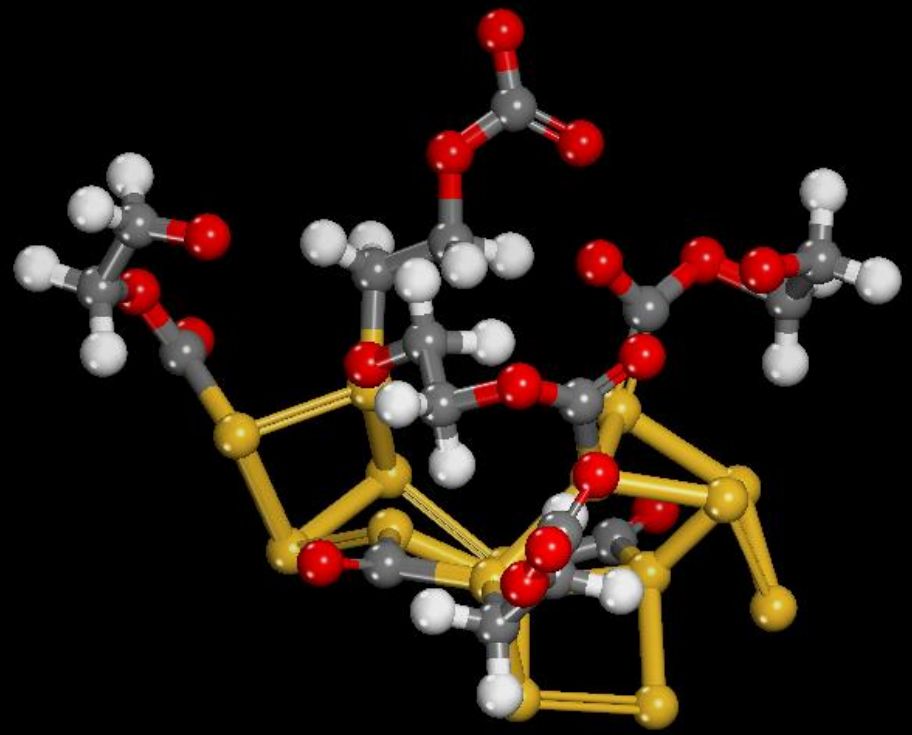
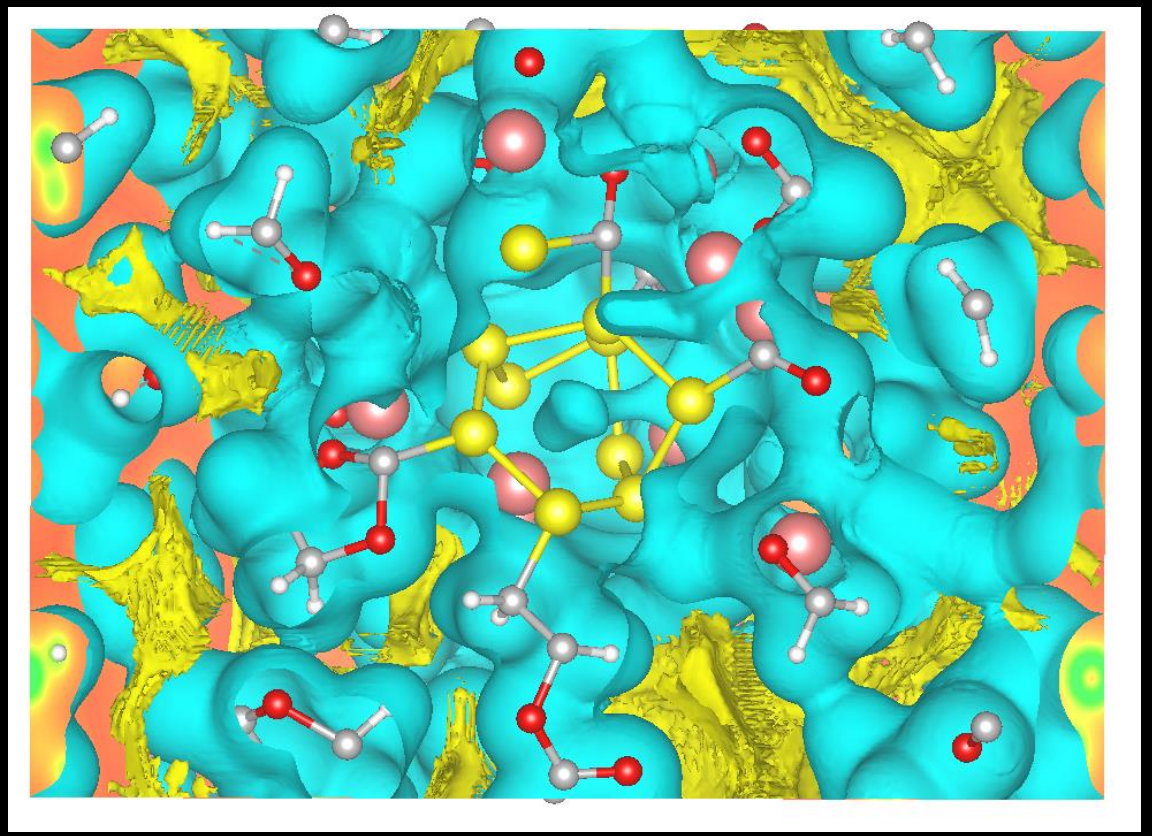
SEI Formation on Si Nanocluster

software: VASP, hardware: ADA, ~60 cores



Initial ethylene carbonate adsorption and decomposition on Si cluster



Electrostatic potential map for Si cluster and solvent decomposition products

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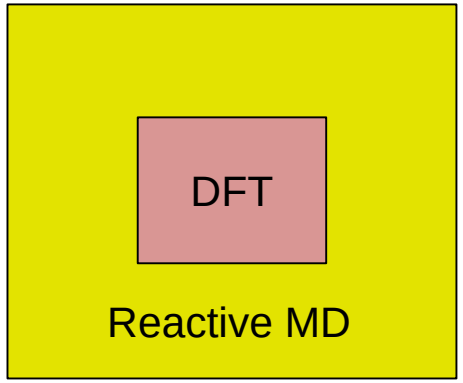
Catalyzed Synthesis of Single-Walled Carbon Nanotubes

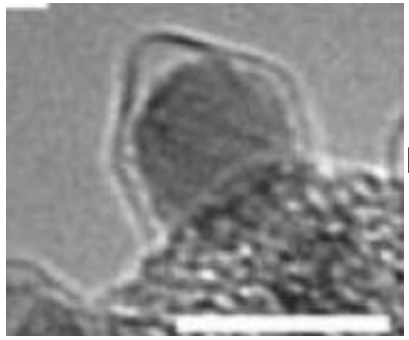
Computational Multiscale Approach



DFT calculations

Small size models: detailed investigation of interatomic interactions, most stable configurations, nature of interactions, minimum energy reaction paths

software: Gaussian09, VASP; our own MD code ;
hardware: Ada, Curie, Brazos



high resolution
tunneling electron microscopy image

Hypothesis:

In this catalytic process, the nanoparticle structure can act as a template to guide nanotube growth toward desired chiralities.

Reactive MD simulations

Larger size models: growth mechanism using DFT-derived parameters. Temperature effects, dynamic-dependent properties, cost-efficient exploration of parameter space

State and evolution of the system dictated by thermodynamic and kinetic factors

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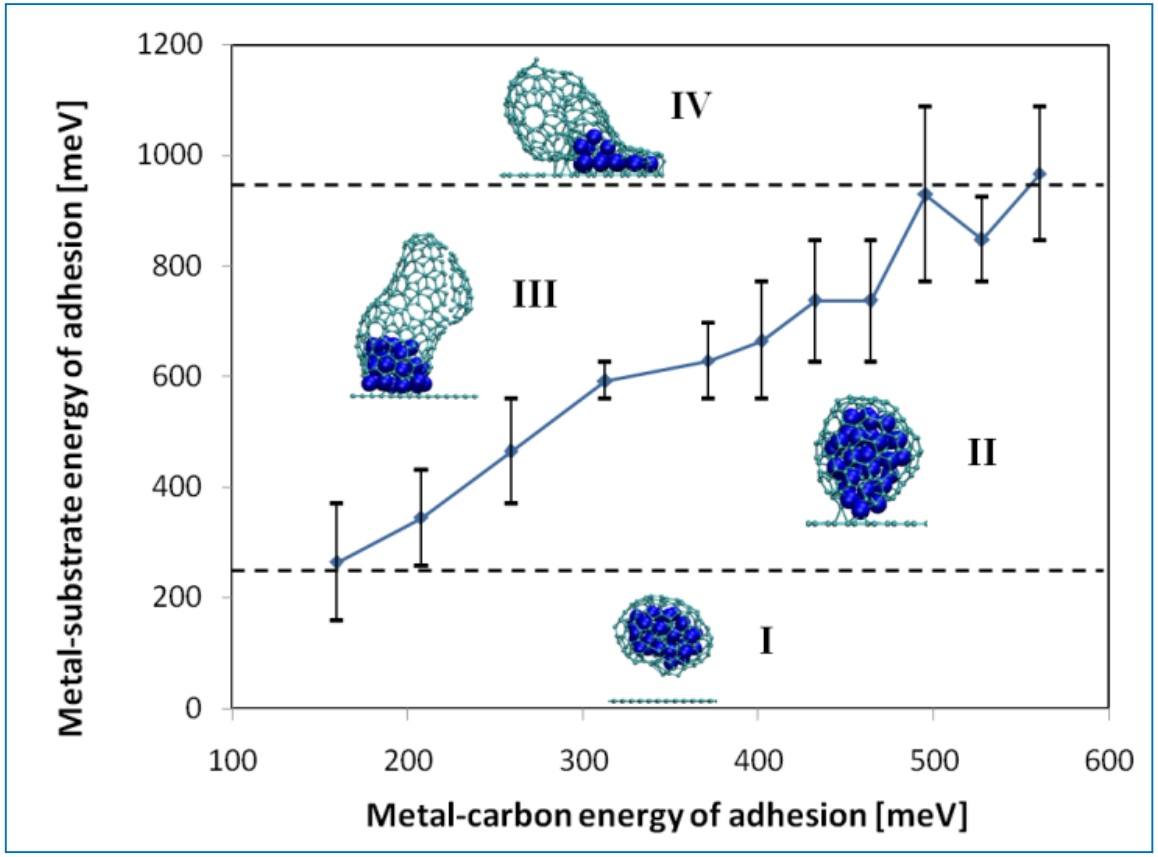
Carbo Nanotube Growth Phase Diagrams



Phase diagrams illustrate regions where high quality (III) or defective tubes may grow (IV) or where the catalyst may become deactivated (I and II)

Accomplished through simulations in high performance computers!!!

software: Reactive MD program developed in Balbuena's group
hardware: EOS, Lonestar, Stampede

Burgos, Jones, Balbuena, JPCC, 118, 4808-4817, 2014

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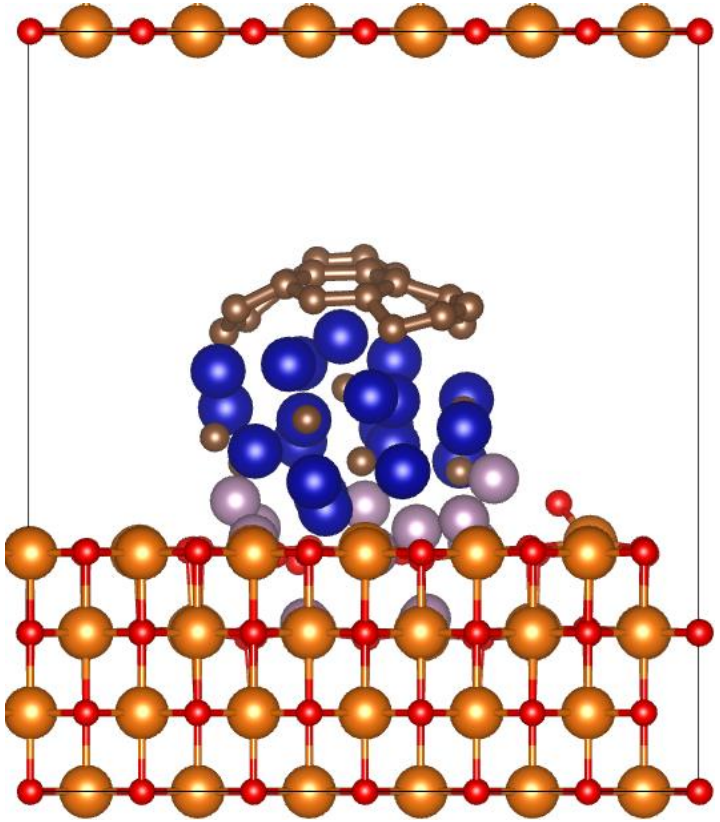
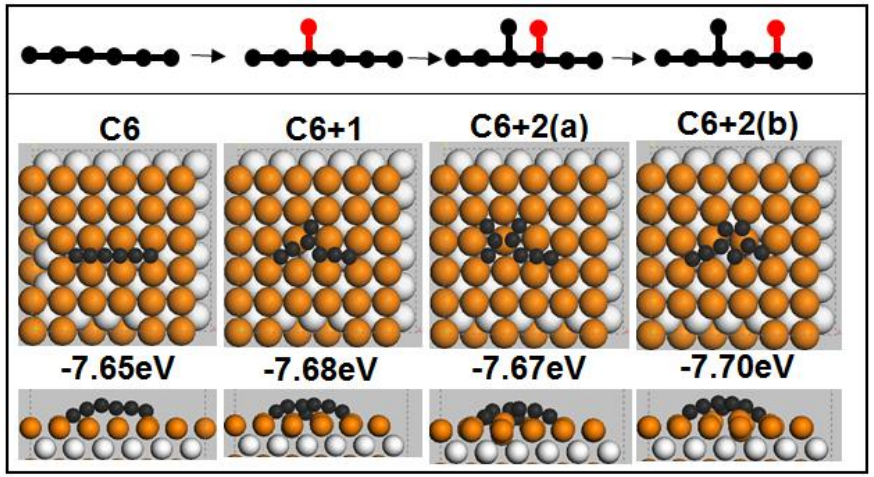
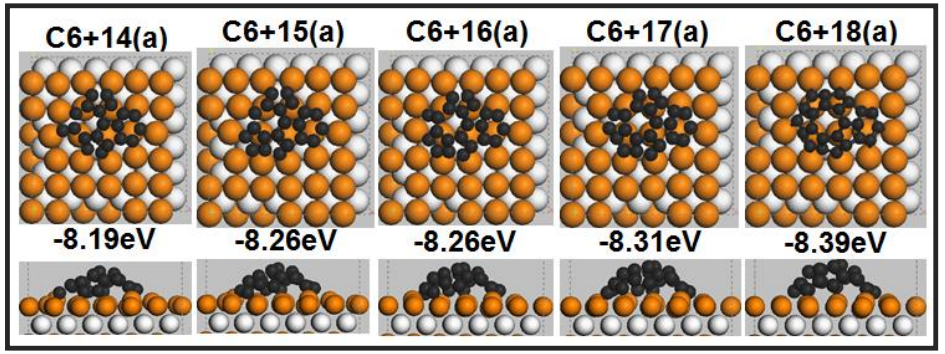
The Study of Graphene/CNT Growth on MgO-Supported Carburized Cobalt Nanoparticles



Thorough study of the CoMoCAT Process used for growing CNT

We explore pathways of growth of graphene on the Cu(100) surface using DFT





software: VASP

hardware: Ada, Curie and Brazos, 120 cores

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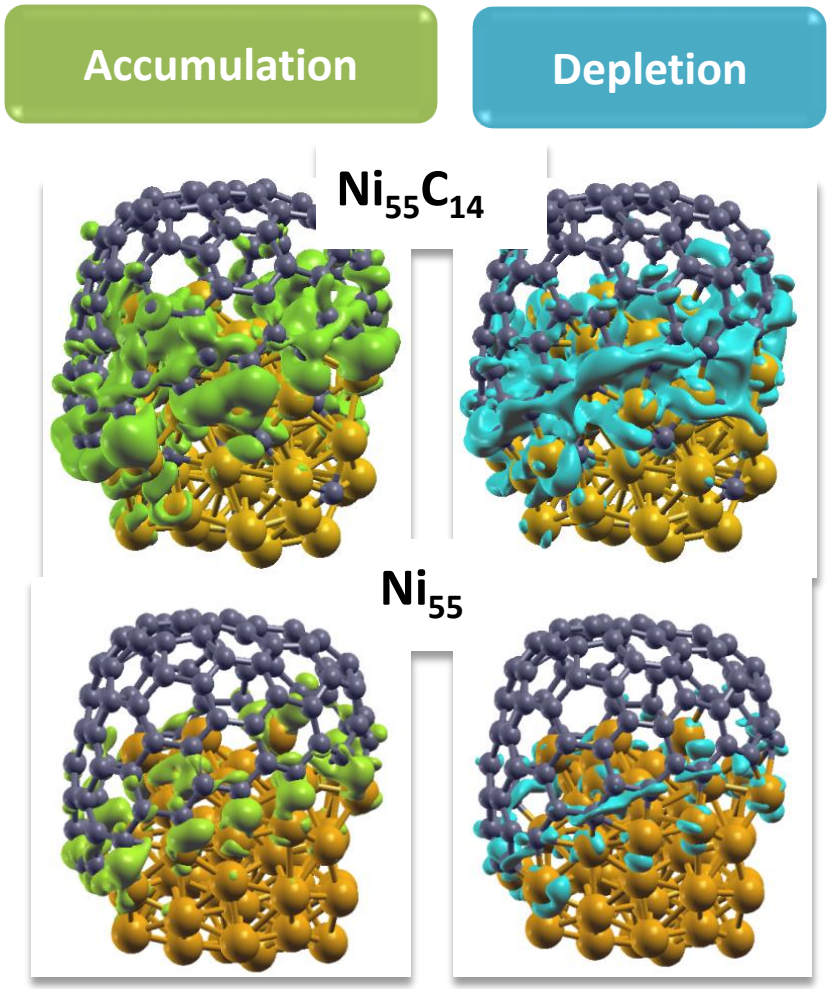
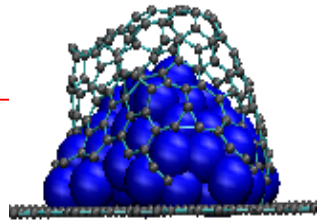
Nucleation and Growth Mechanisms of Single-Walled Nanotubes on Carbide and Metal Nanoparticles



- Electron density transfer between growing nanotube and catalytic nanoparticle calculated using DFT in VASP®
- Simulation consisted of 55 Ni Atoms and 100+ C atoms and was ran in parallel on Ada ~80 CPUs

- Reactive Molecular Dynamics simulation demonstrating the catalytic growth process
- SIMCAT Fortran code
- Code ran in 1 CPU for 600+ hours



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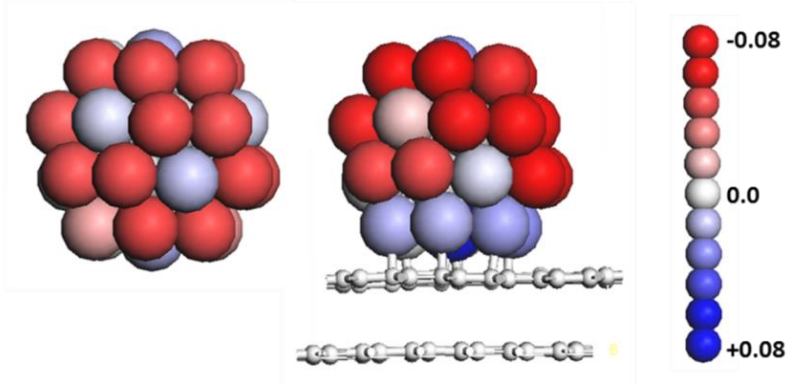
Catalyst Supported on a Substrate: Charge Transfer

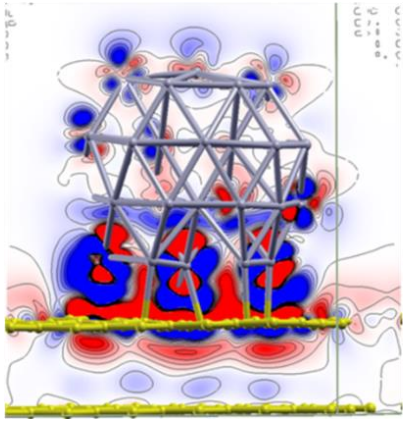
Bader Charges: After adsorption, on the interface the charge of the atoms is positive, on the top is more negative.

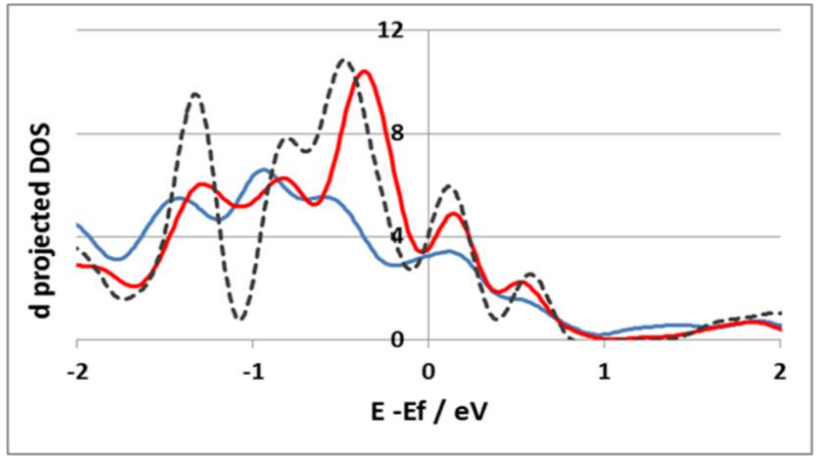


J. Ma, G. Ramos-Sanchez,
PB Balbuena, N. Alonso-Vante et al,
ACS Catalysis, 3, 1940-1950, (2013)

Details of the electronic transfer during reaction and the effect of the catalyst support (carbon) incorporated to the DFT simulations

Total effect: The high hybridization, modification of the structure and charge transfer lead to more states near the Fermi level of top atoms, the DOS of these atoms are shifted closer to the Fermi level.





Accomplished through simulations in high performance computers!!!

software: VASP;
hardware: EOS, Stampede

G. Ramos-Sanchez and P. B. Balbuena, PCCP, 15, 11950-11959, (2013)

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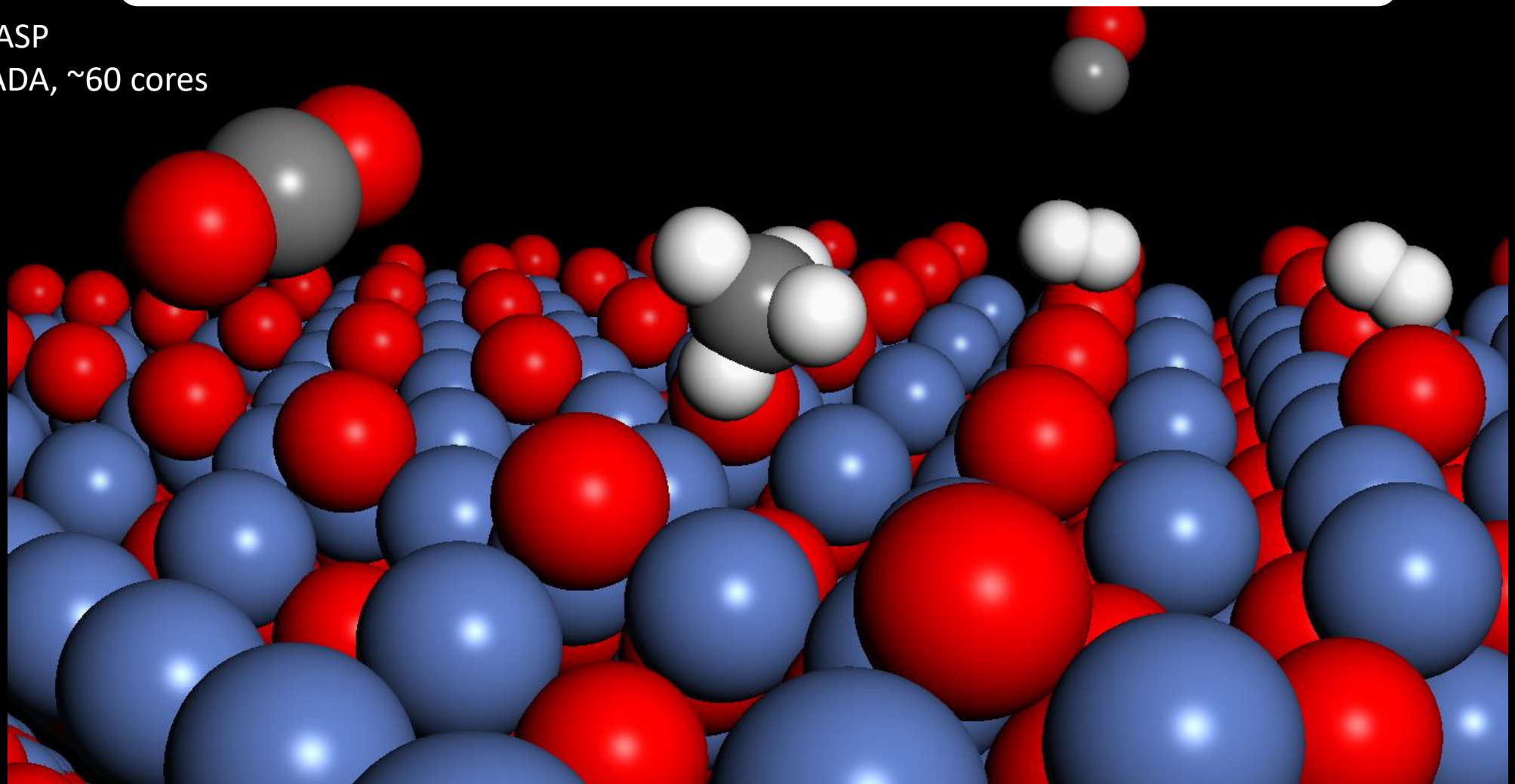
Project: Coke-resistant catalysts for the dry reforming reaction of CH_4

Figure: NiO(111)-*p*(2x2) octopolar surface which exhibits coke resistant property

software: VASP
hardware: ADA, ~60 cores



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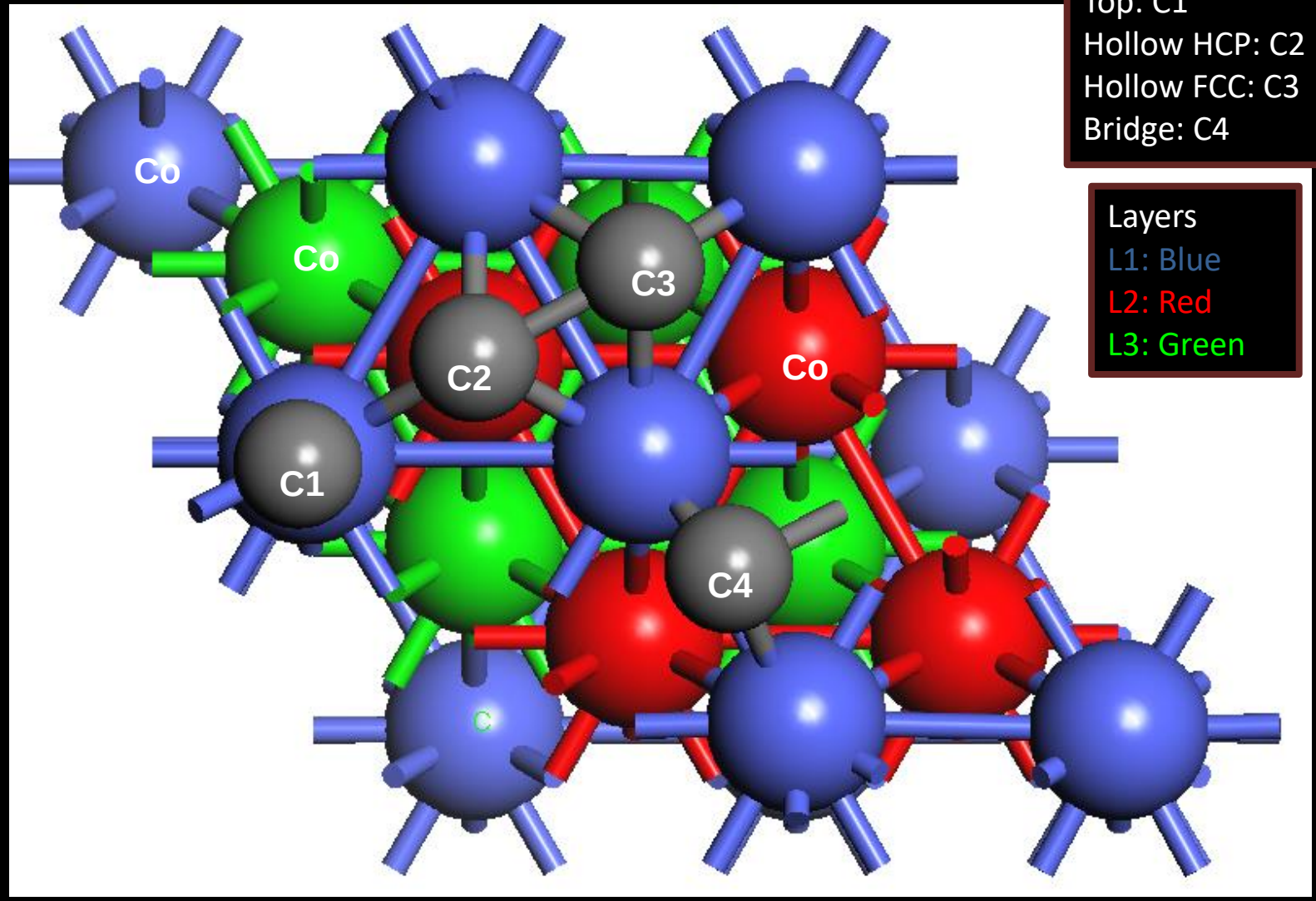
Carbon adsorption test for SWCNT growth using VASP



Sites
Top: C1
Hollow HCP: C2
Hollow FCC: C3
Bridge: C4

Layers
L1: Blue
L2: Red
L3: Green

software: VASP
hardware: ADA,
~60 cores

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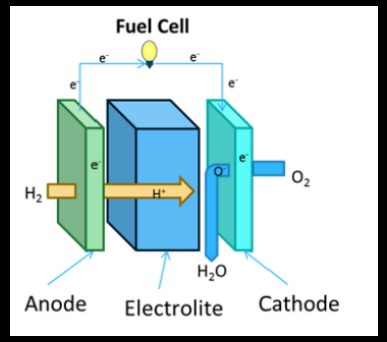
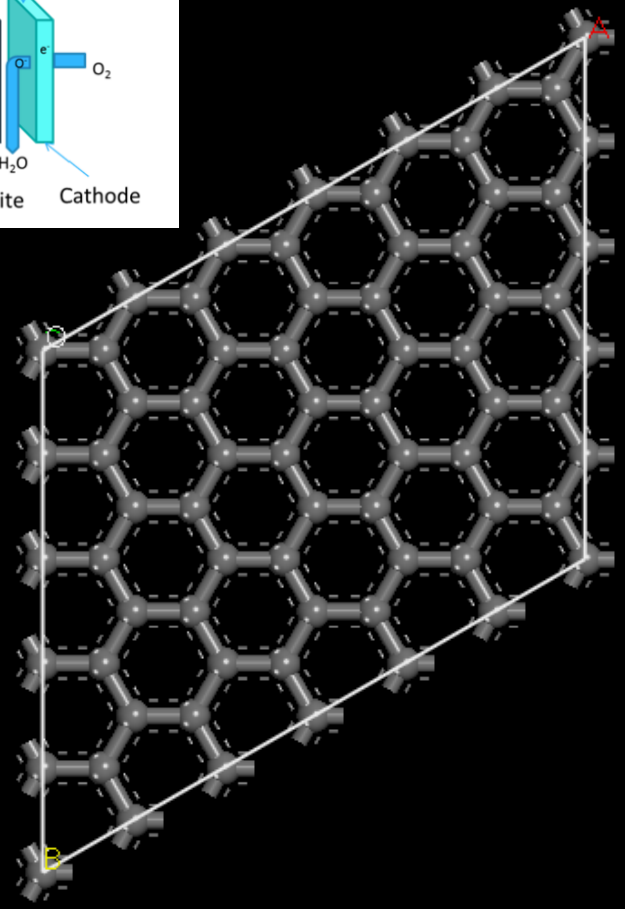
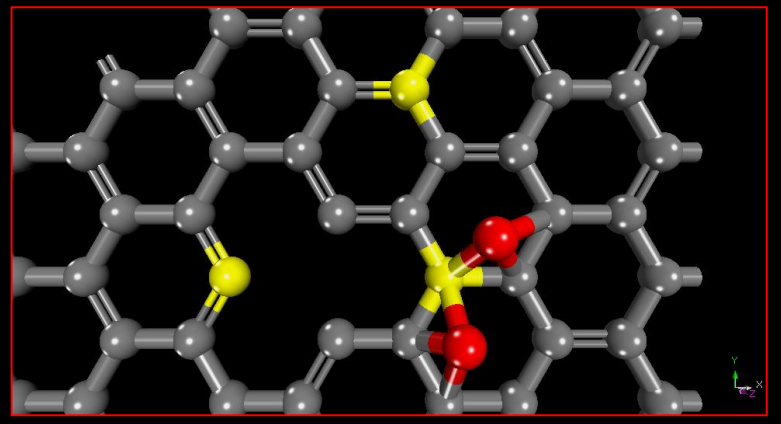
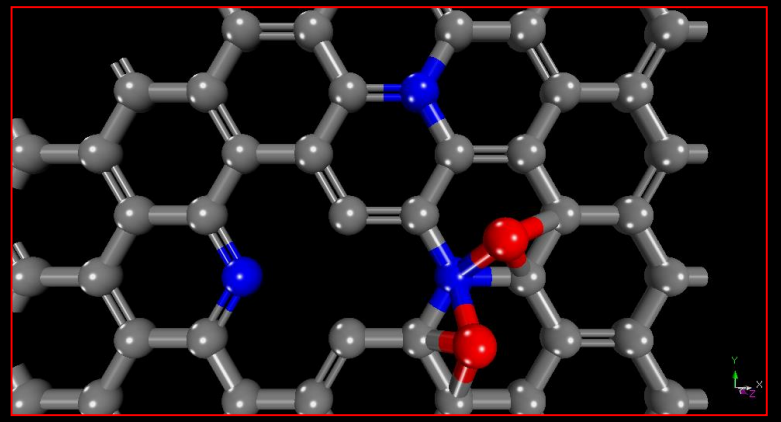
Modeling Electrochemical Reactions on Nanostructured Carbon Materials









software: VASP
hardware: ADA, ~60 cores

- Nitrogen
- Sulfur
- Oxygen

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Acknowledgements

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Prof. Partha Mukherjee (TAMU)
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Dr. Kevin Leung (Sandia Nat. Lab)
Dr. Susan Rempe (Sandia Nat. Lab)
Dr. Chunmei Ban (NREL)
Dr. Omar Solorza (Cinvestav, MX)
Dr. N. Alonso-Vante (U Poitiers)
Dr. Avetik Harutyunyan (HRI)
Dr. Renu Sharma (NIST)
Dr. Fadwa El-Mellouhi (QEERI)

DOE/EERE
DOE/BES
Honda Research Institute
National Science Foundation
Qatar National Research Foundation

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NERSC
HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY
Brazos HPC Cluster
TACC TEXAS ADVANCED COMPUTING CENTER
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THE UNIVERSITY OF TEXAS AT AUSTIN