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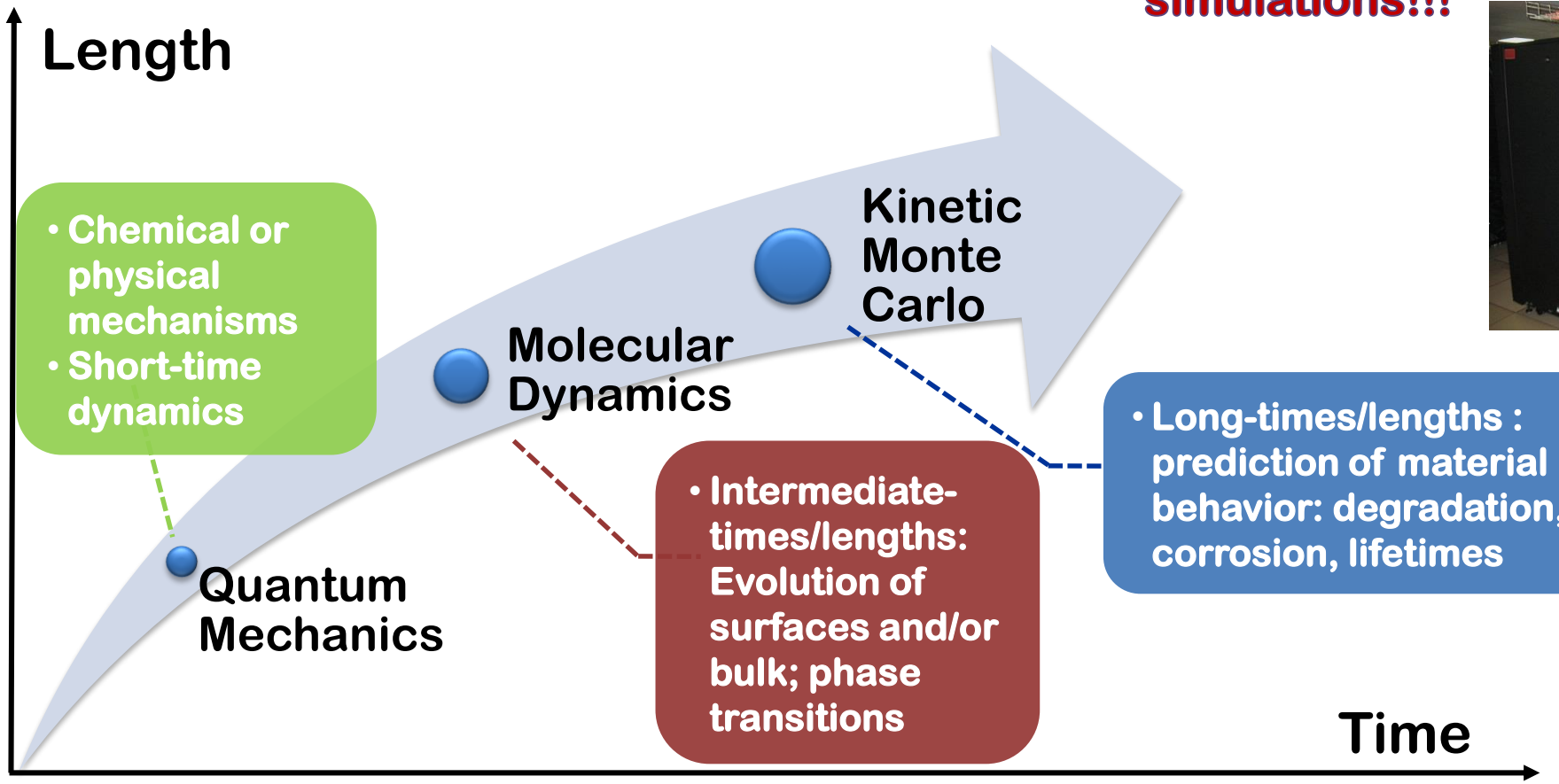
First-principles multiscale analysis

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

Accomplished through high performance computer simulations!!!



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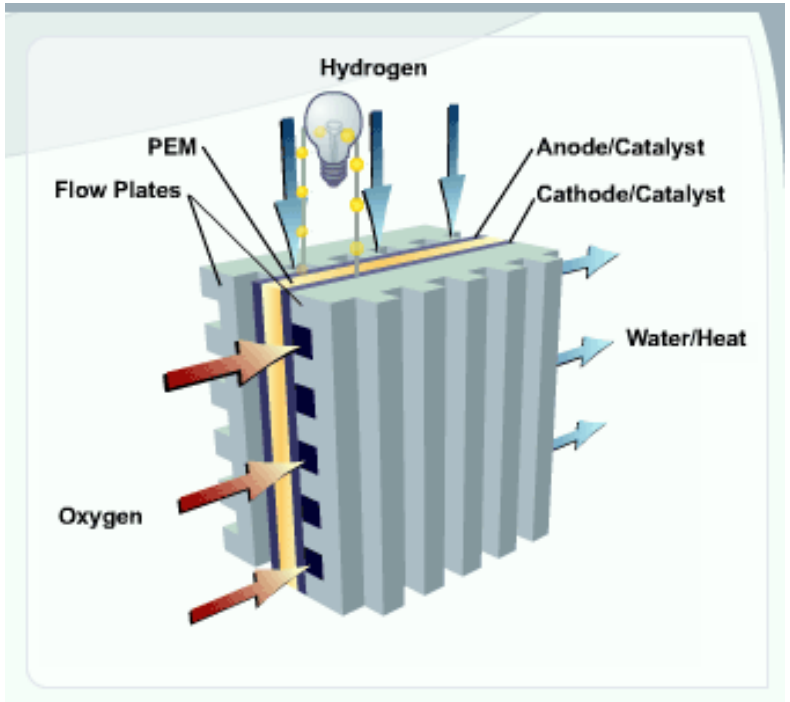
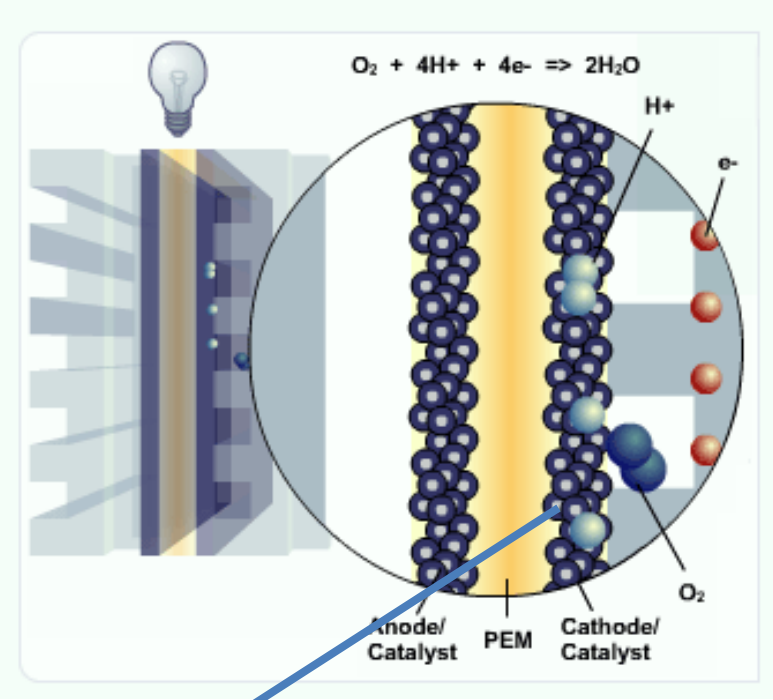
Producing electricity from fuel cells requires active and stable electro-catalyst materials

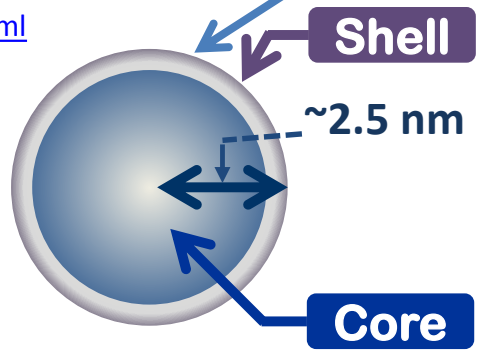


Taken from:
http://www.fueleconomy.gov/feg/animation/mod1.html



Challenge:
test and design the appropriate material for the electro-catalyst:

Accomplished through simulations in high performance computers!!!



tiny metallic electro-catalysts (nanometers) need to survive in acid medium

oxygen reacts with protons and electrons over an electro- catalyst and is converted into water, while in the other electro-catalyst hydrogen is dissociated into protons and electrons

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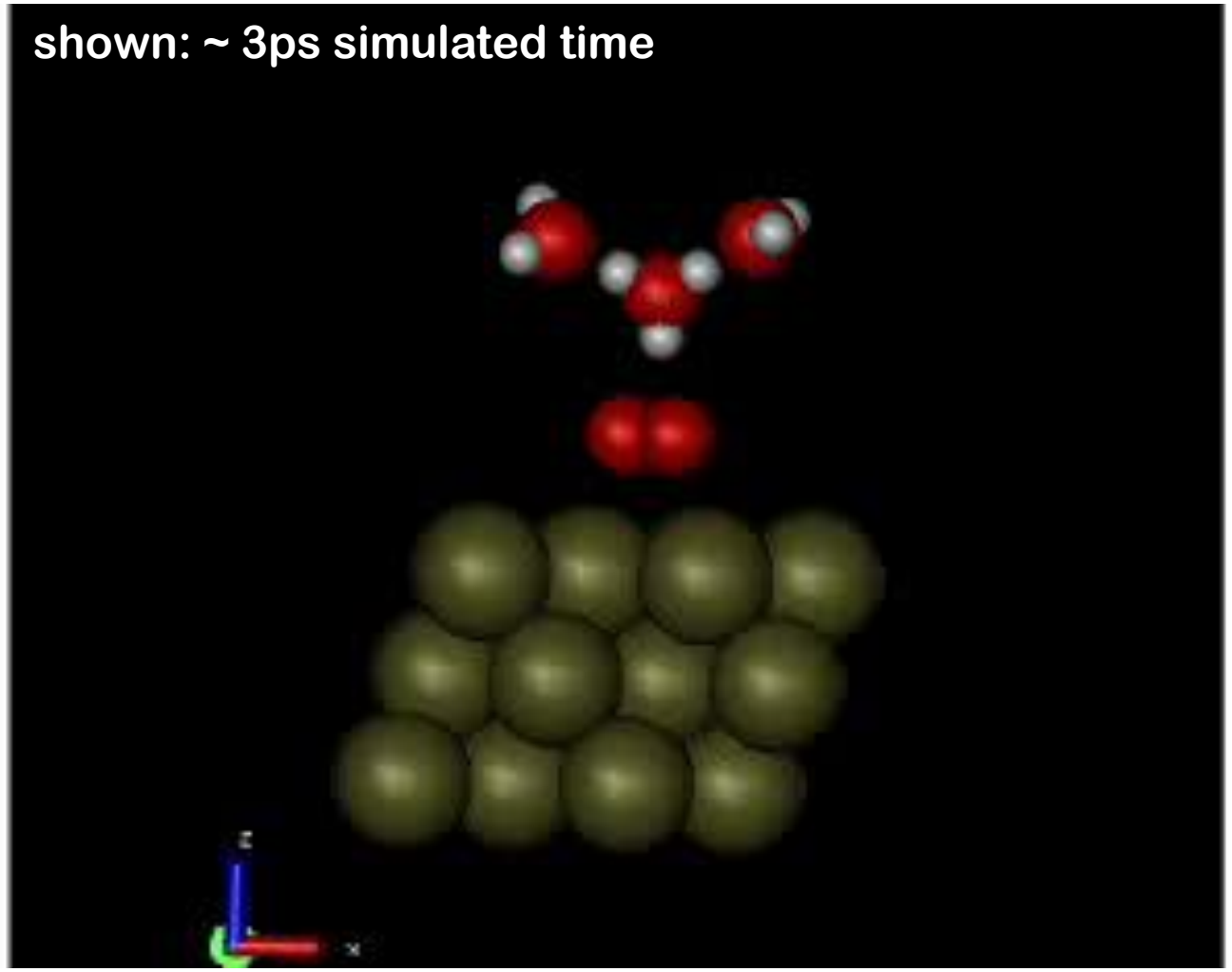
What can be learned from density functional theory (DFT) and ab initio molecular dynamics (AIMD) simulations



Oxygen (red) dissociates in presence of water and protons on the surface of tiny fuel cell platinum electro-catalysts

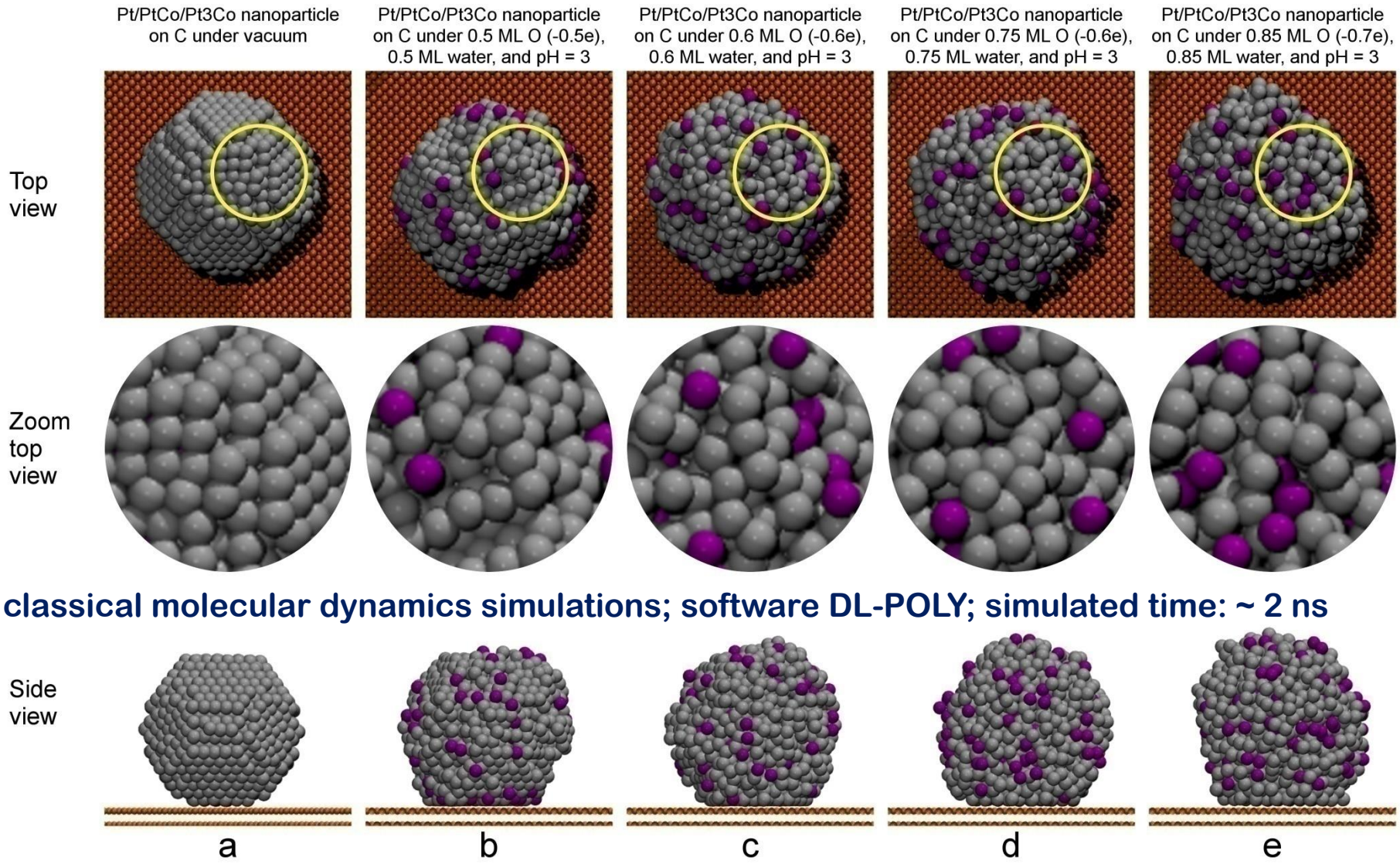
Adsorption Desorption Reaction

Accomplished through DFT and AIMD simulations in high performance computers!!!

Software: VASP
Hardware: ADA, ~60 cores

Balbuena's group, TAMU

Oxidation of $Pt/PtCo/Pt_3Co$ nanoparticle



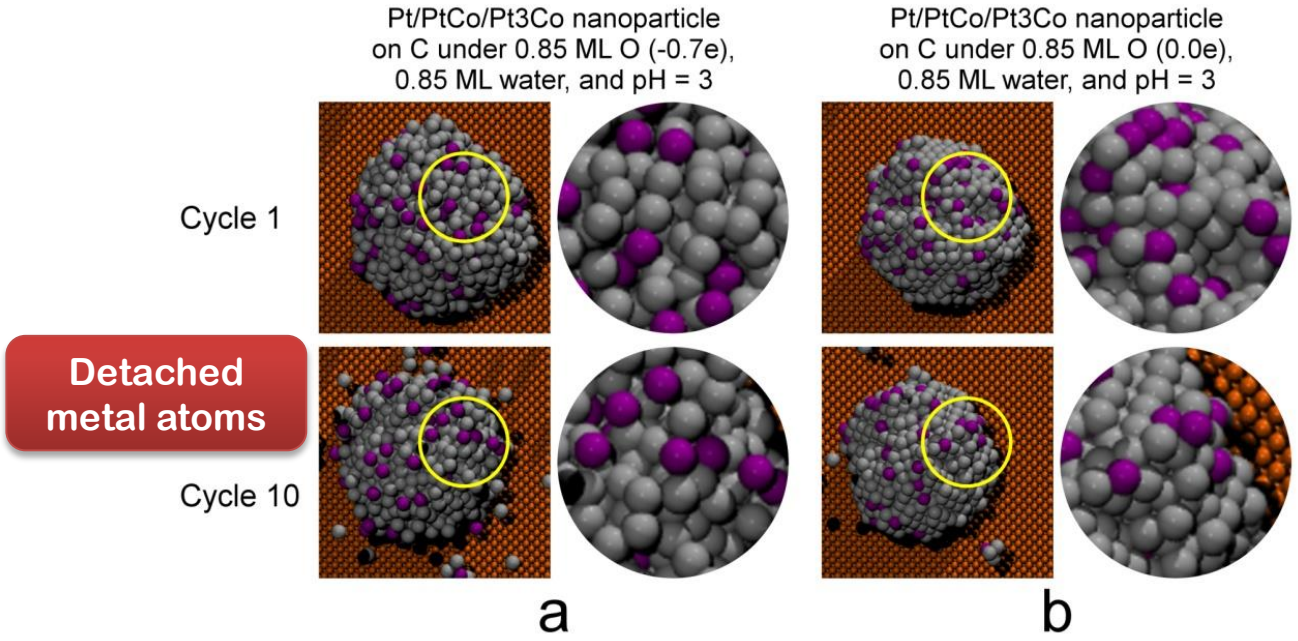
classical molecular dynamics simulations; software DL-POLY; simulated time: ~ 2 ns

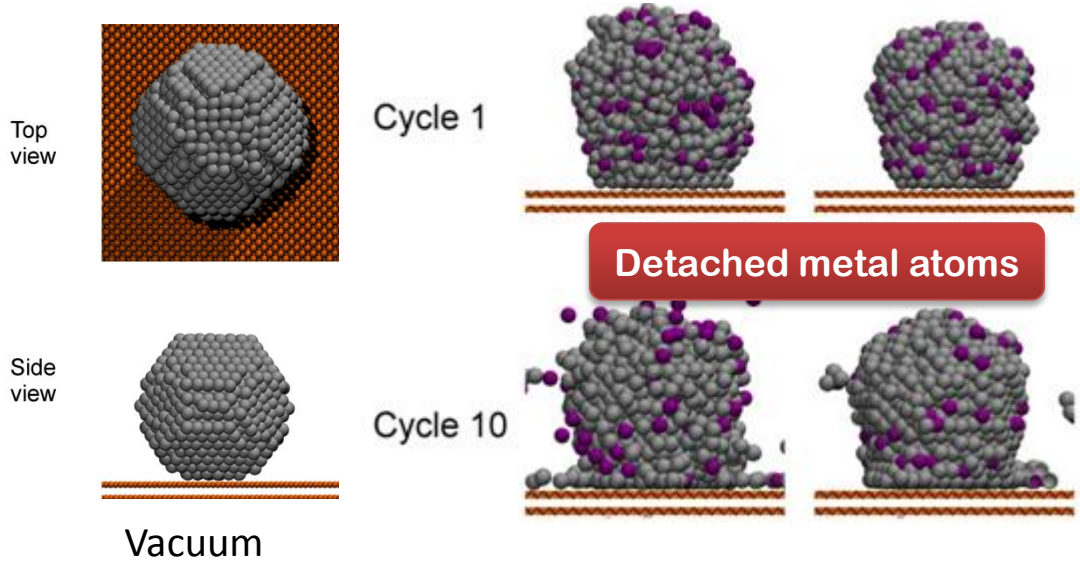
Adsorbates are not shown

Increase oxygen coverage

evolution of the electro-catalyst particle in longer times

Degradation of nanoparticles with cycling





Accomplished through simulations in high performance computers!!!

- **Metal atoms dissolve after cycling**

Adsorbates are not shown

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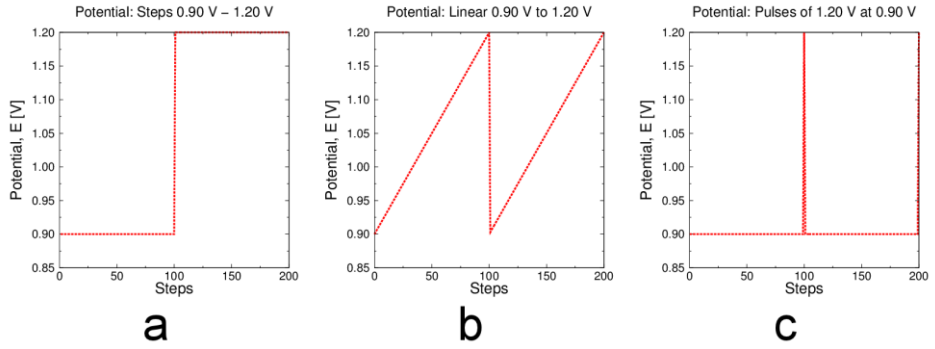
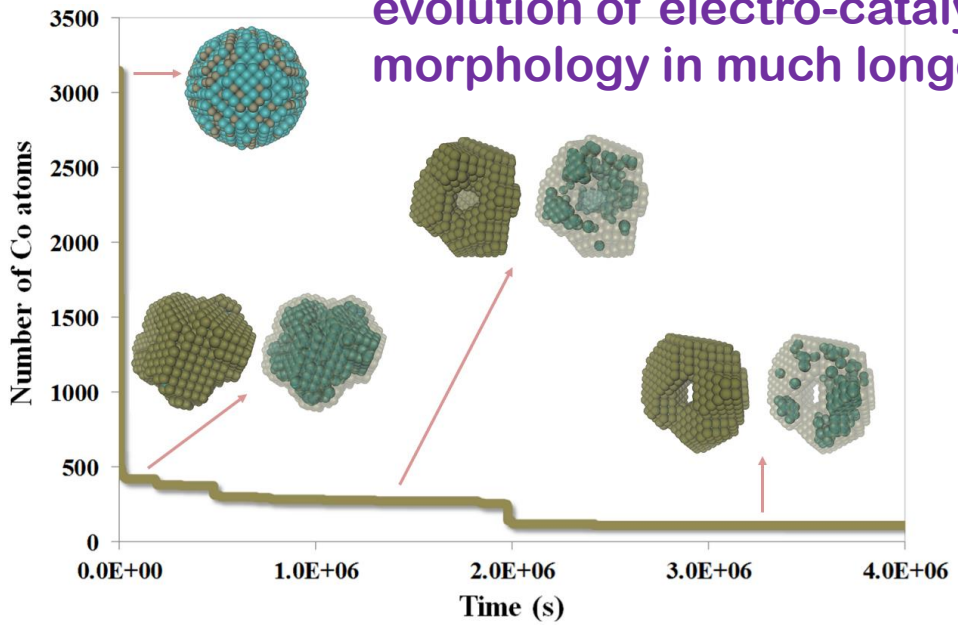
Variable potential KMC simulations



Kinetic Monte Carlo (KMC) simulations (code written by R. Callejas-Tovar, TAMU)

evolution of electro-catalyst morphology in much longer times!!!



Balbuena et al, Electrochimica Acta, 2013

While driving a fuel-cell car, there are changes in the conditions in which our electrocatalyst operates

Accomplished through simulations in high performance computers!!!

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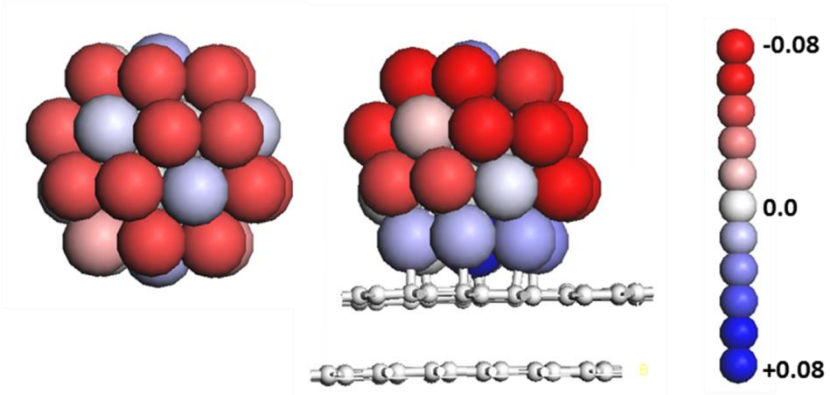
Catalyst supported on a substrate: charge transfer

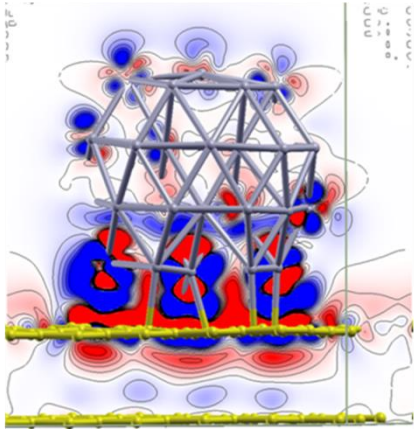
Bader Charges: After adsorption, on the interface the charge of the atoms is positive, on the top is more negative.

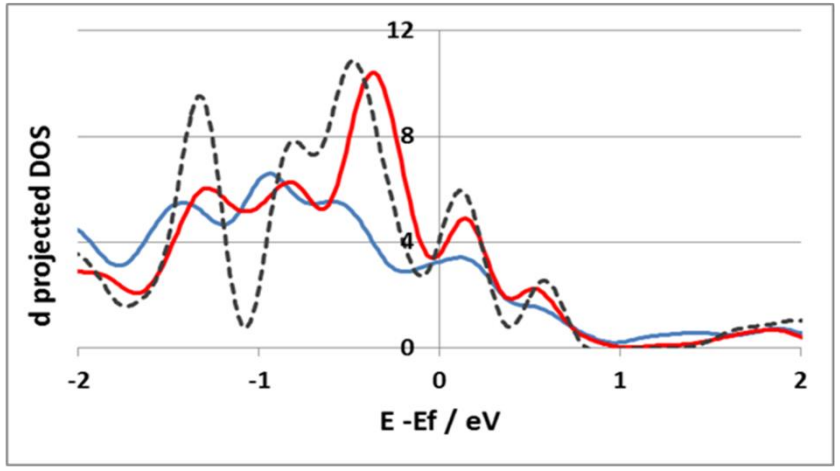


J. Ma, G. Ramos-Sanchez,
PB Balbuena, N. Alonso-Vante et al,
ACS Catalysis, 3, 1940-1950, (2013)

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)

Computational Materials Design for Catalysis and Renewable Energies

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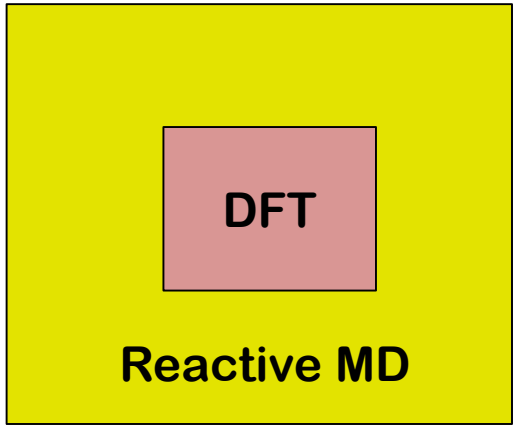
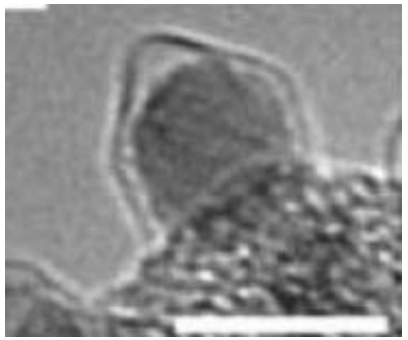
Catalyzed Synthesis of Single-Walled Carbon Nanotubes

Computational Multiscale Approach





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.

DFT calculations

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

Reactive MD simulations

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

Software: Gaussian09, VASP; our own MD code ;
Hardware: EOS, Lonestar, Stampede

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

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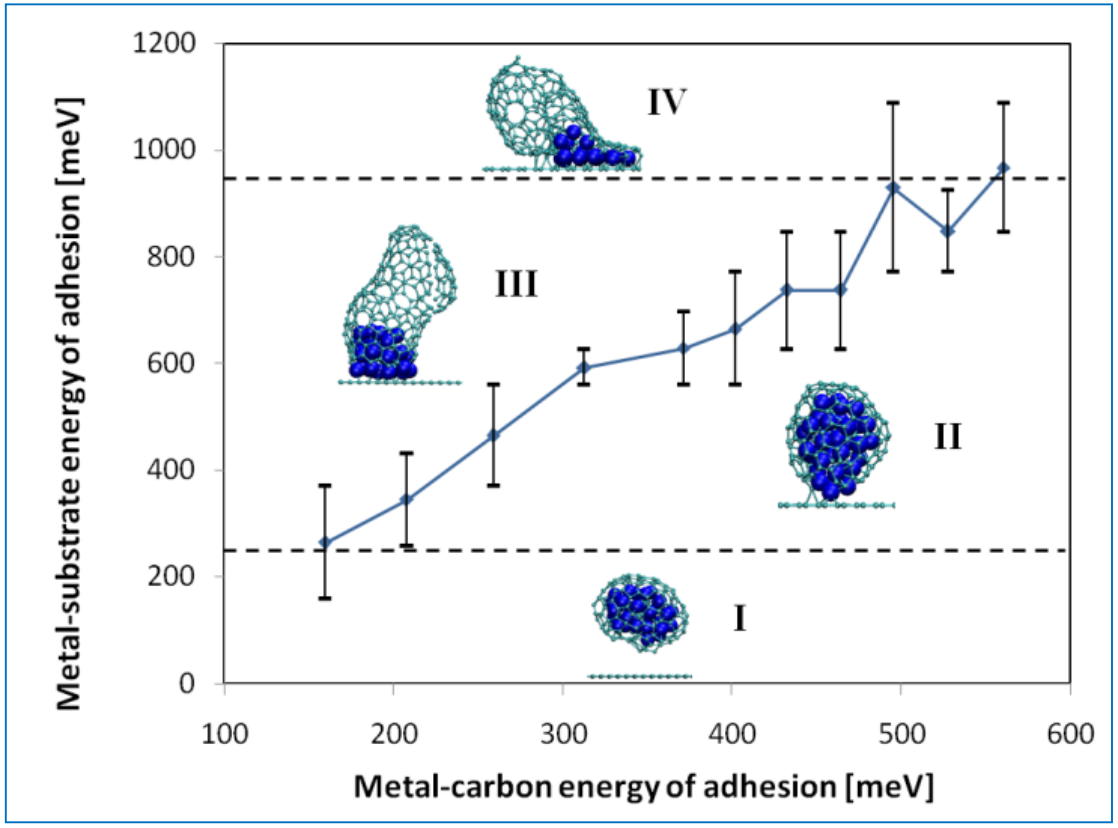
Carbon nanotube growth phase diagrams



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!!!

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

Software: Reactive MD program developed in Balbuena's group
Hardware: EOS, Lonestar, Stampede

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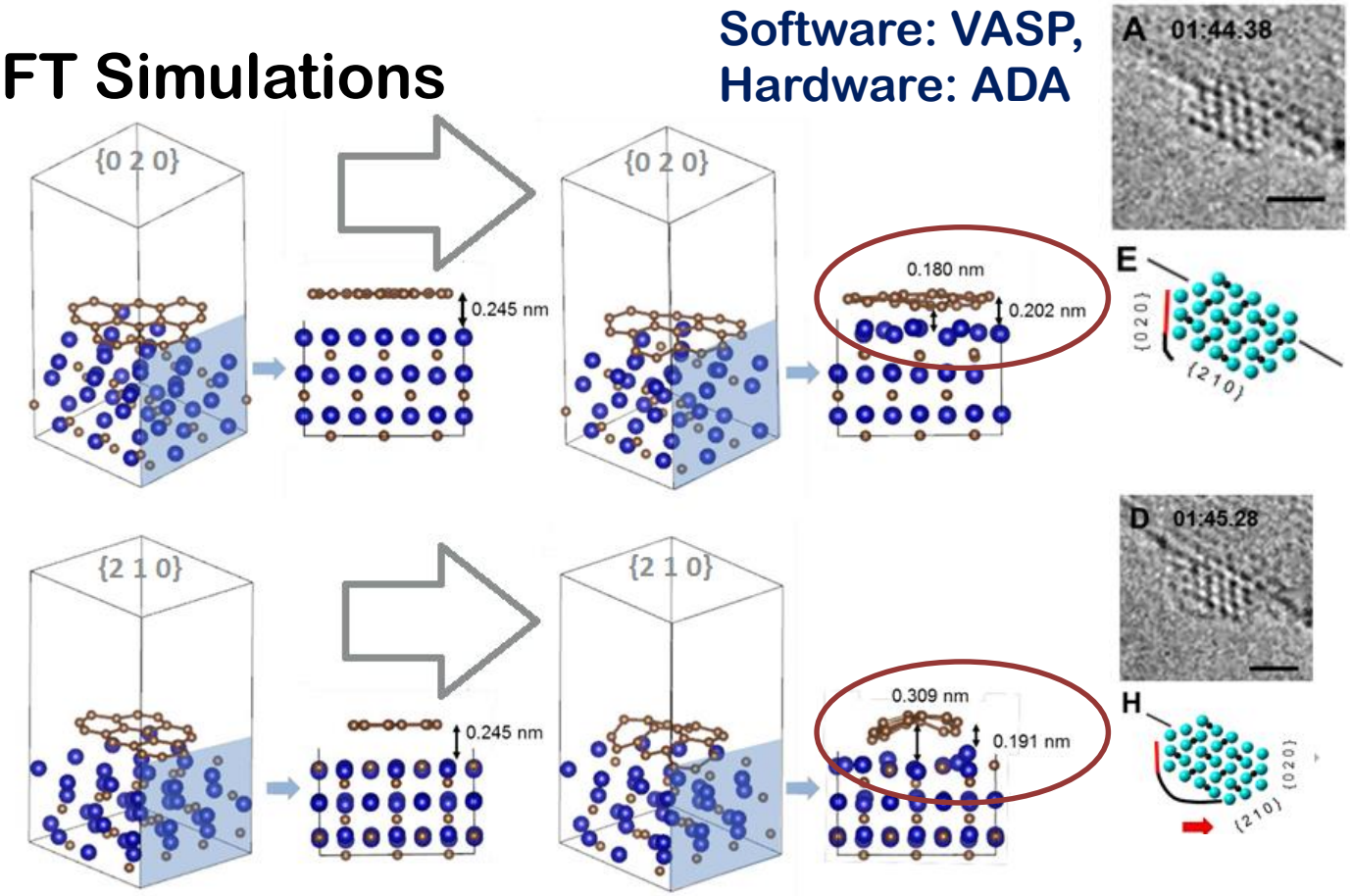
Combined computational and experimental approach

DFT Simulations

Software: VASP,
Hardware: ADA

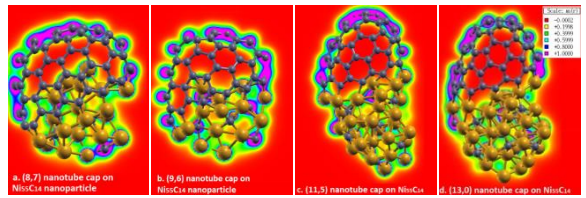


Picher, M., Lin, P.A., Gomez-Ballesteros, J.L., Balbuena, P.B., Sharma, R.. *Nano Letters*, 2014. **14**(11): p. 6104-6108

New insights about carbon nanostructure growth

Accomplished through simulations in high performance computers!!!

Software: Gaussian 09, VASP;
Hardware: ADA



Gomez-Ballesteros and Balbuena, *PCCP*, 17, 15056-15064, (2015)

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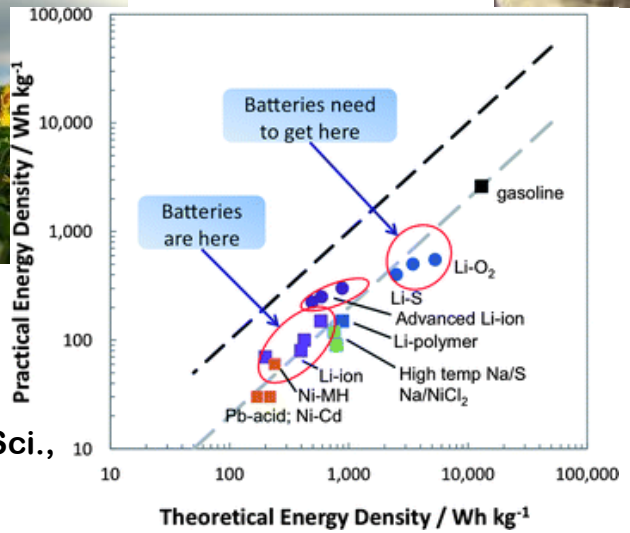
Renewable energies (solar, wind) are intermittent

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)

Computational Materials Design for Catalysis and Renewable Energies

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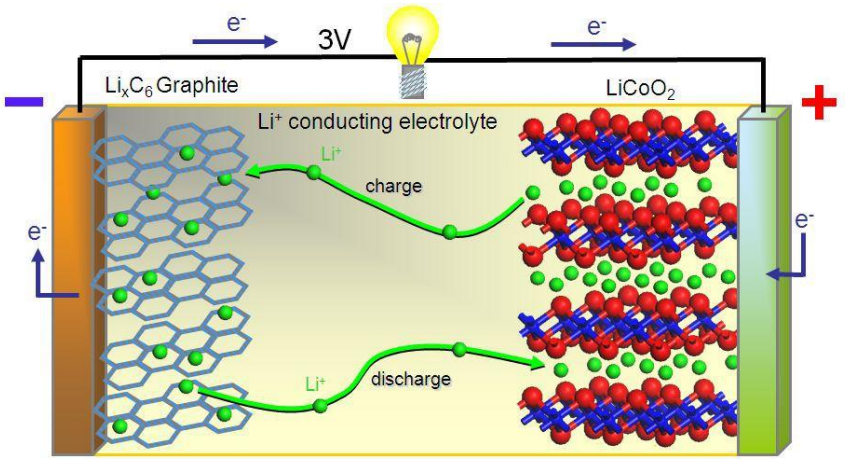
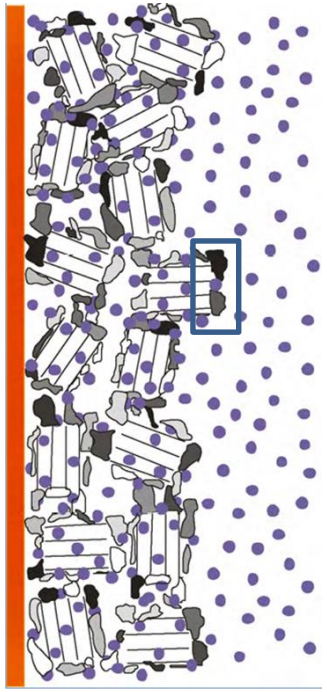
Lithium-ion

for small devices

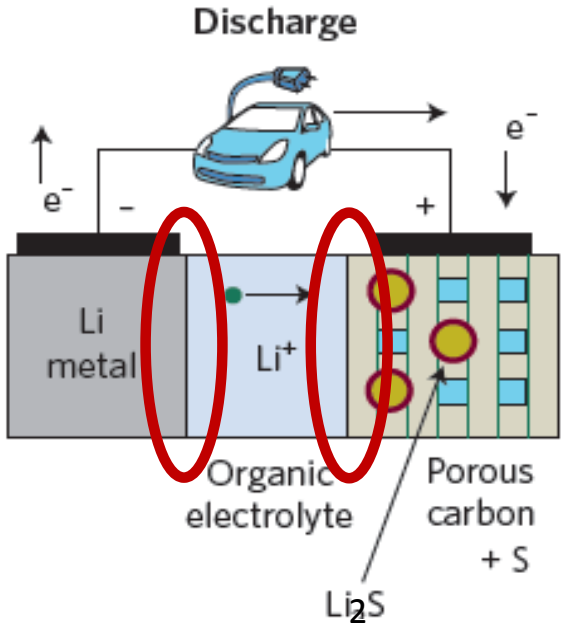




interfacial reactions generate a multicomponent solid-electrolyte interphase (SEI) film. Its properties are key for the battery lifetime

Lithium-Sulfur

for electric cars



higher energy density but complex chemistry

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

Software: Gaussian 09, VASP;
Hardware: ADA

Balbuena's group, TAMU

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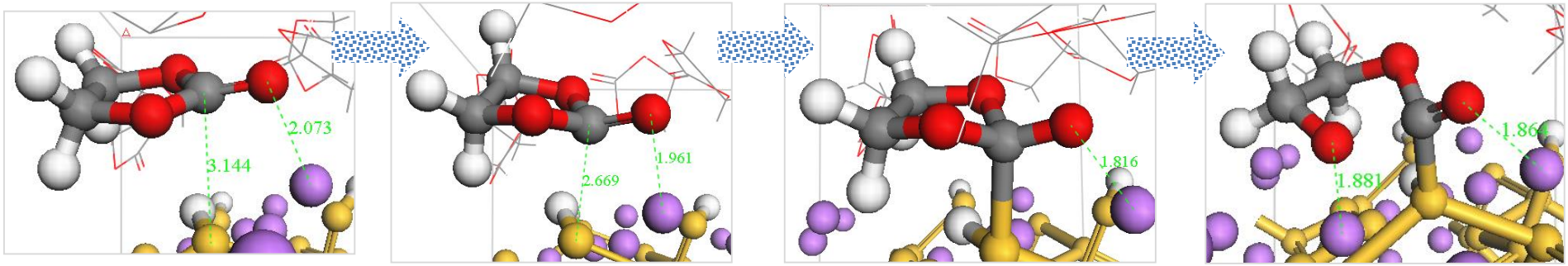
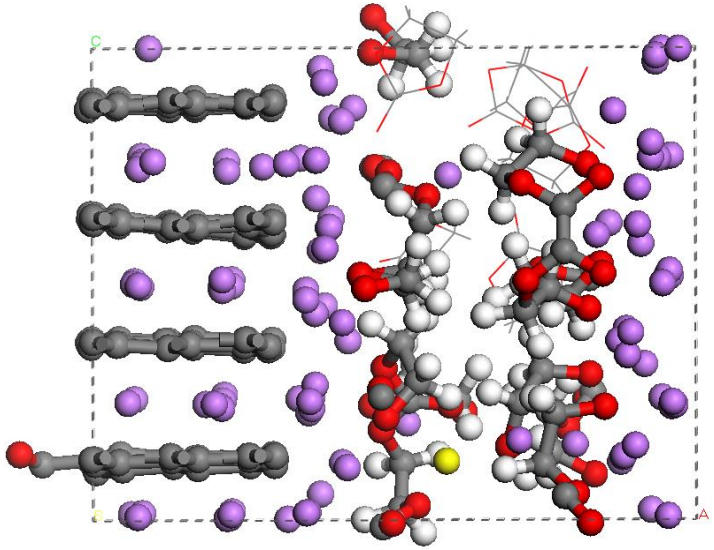
SEI reactions on nanostructured carbon and Si anodes of Li-ion batteries

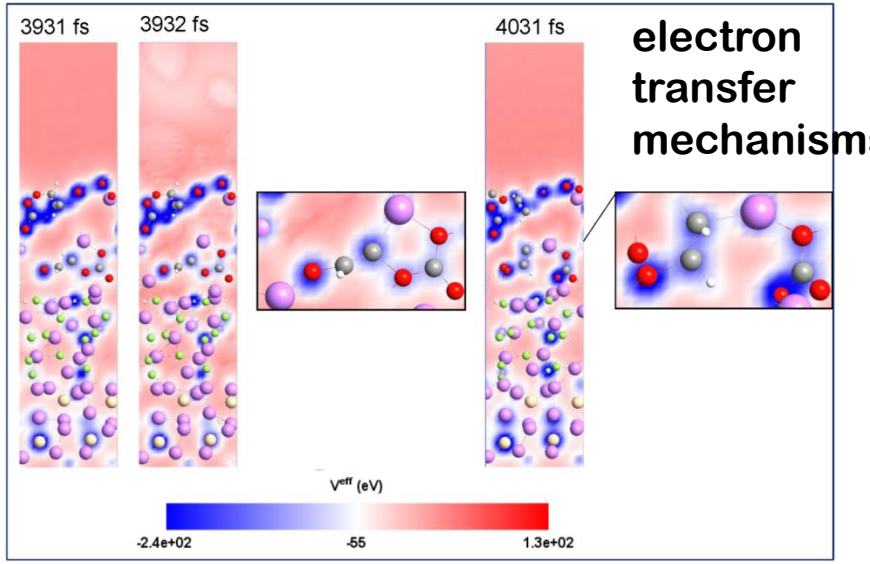


-0.22 e **-0.63 e** **-1.12 e** **-1.56 e**

J. M. Martinez de la Hoz, K. Leung and P. B. Balbuena, ACS Appl. Mat. and Interfaces, 2013



effects of surface termination, surface area, nano-architecture…



FA Soto, JM Martinez, JM Seminario, PB Balbuena, Chem. Mater.

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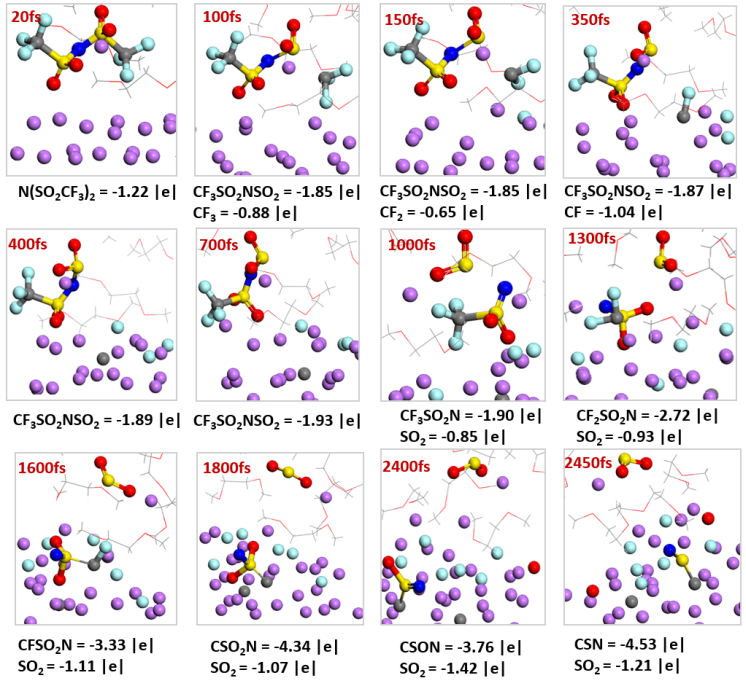
The complex and interconnected chemistry of Li-S batteries



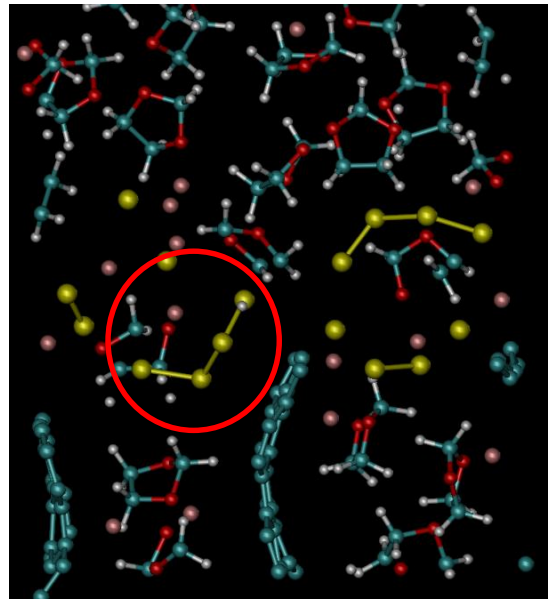
multiple electrolyte decomposition reactions at the surface of the Li metal anode identified by AIMD simulations

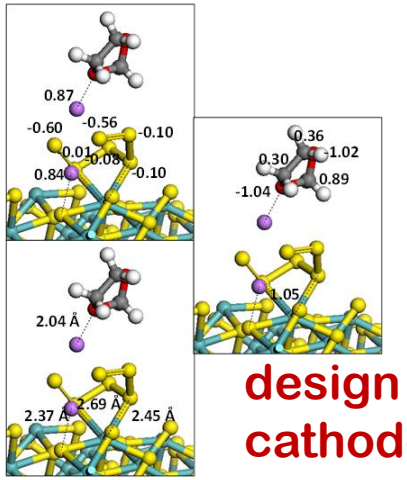
LE Camacho-Forero, T Smith, S Bertolini, PB Balbuena, JPCC, under review

Software: Gaussian 09, VASP;
Hardware: ADA

Sulfur lithiation reactions at the C/S composite cathode: effect of small carbon pores studied with DFT and AIMD

JC Burgos and PB Balbuena, work in progress





design of alternative cathode materials

E Kamphaus and PB Balbuena, work in progress

Accomplished through simulations in high performance computers!!!

Computational Materials Design for Catalysis and Renewable Energies

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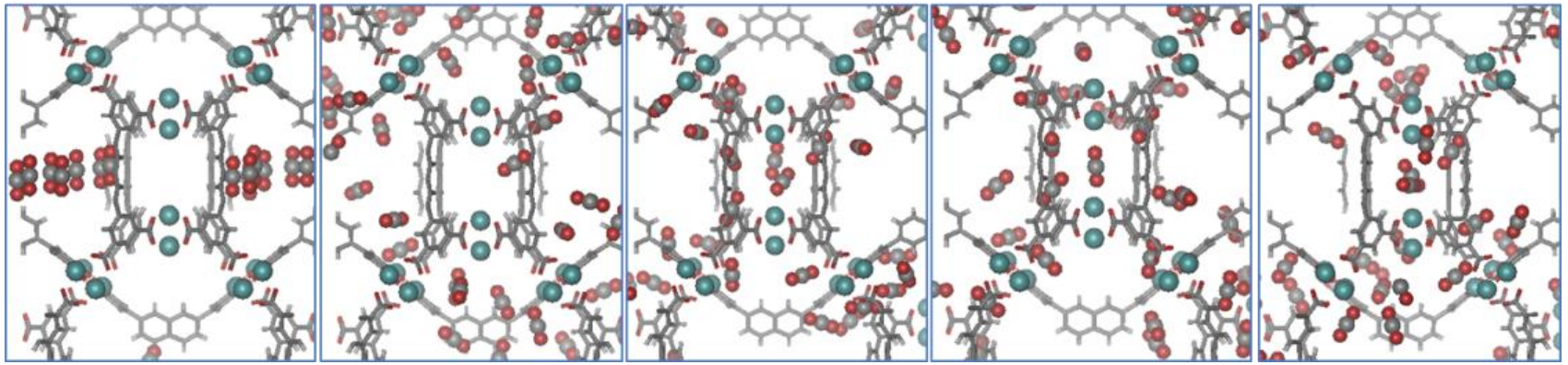
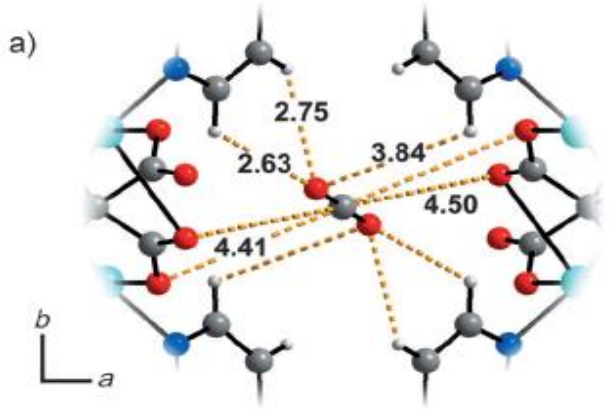
CO_2 storage for cleaner environments

New material for CO_2/N_2 separations from flue gas streams

DFT and AIMD study of CO_2 captured in molecular trap



Li, Yu, Lu, Sun, Sculley, Balbuena, and Zhou, Nat. Comm., 2013



multipoint interaction pocket

Heat of adsorption (zero coverage) = -44 Kj/mol
Not too weak (high selectivity), not too strong (low regeneration cost)

Wriedt, Sculley, Yakovenko, Ma, Halder, Balbuena and Zhou, *Angew. Chem. Int. Ed.*, 2012

Accomplished through combined experimental/ computational studies in high performance computers!!!

Software: Gaussian 09, VASP;
Hardware: EOS, ADA, Stampede

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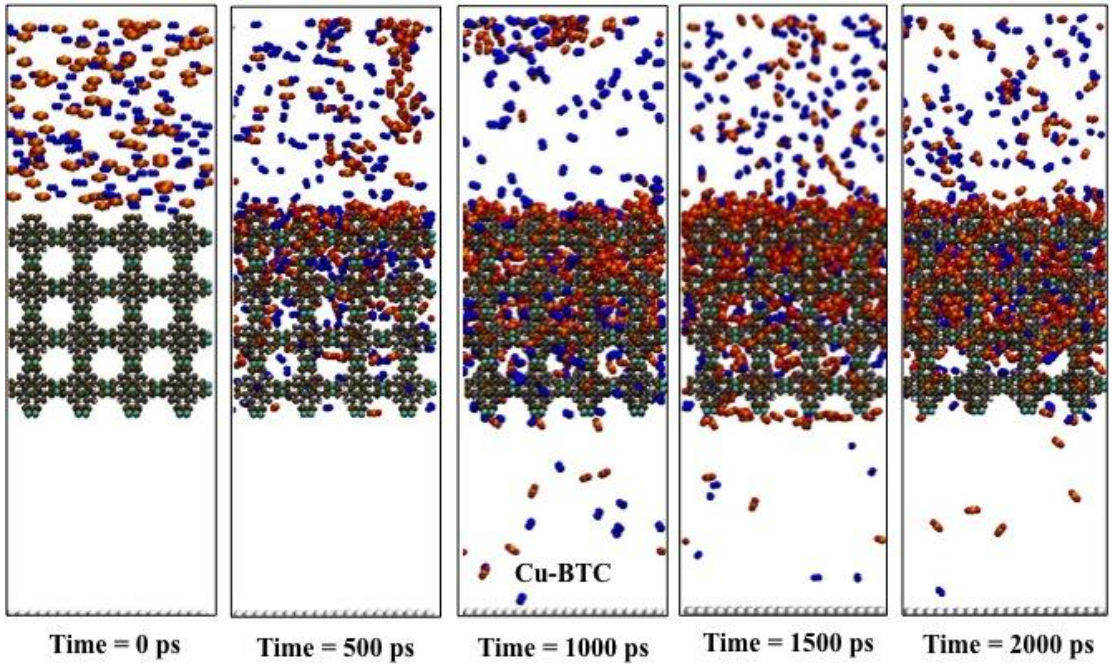
CO_2 storage for cleaner environments

Membrane simulation



Once an efficient material has been identified for gas storage or separations, a membrane is fabricated. The mixture of gases passes through the membrane and selectively one of the gases is trapped. Here we simulate membrane operation at the actual pressure and temperature conditions

F Cabrales Navarro, JL Gomez-Ballesteros, PB Balbuena, J. Memb. Sci., 2013

Software: DL-POLY and our own MD programs; Hardware: EOS

Accomplished through molecular simulations in high performance computers!!!

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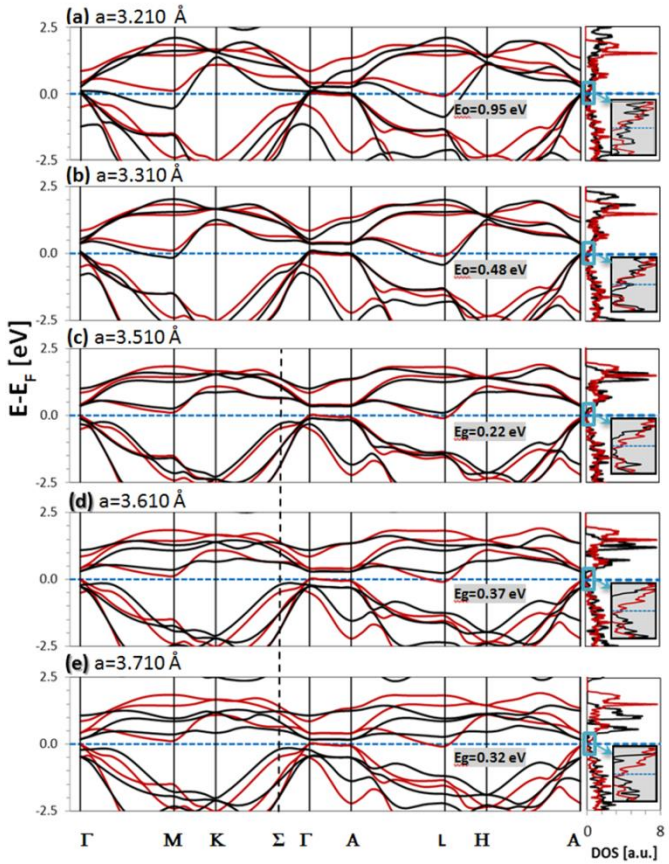
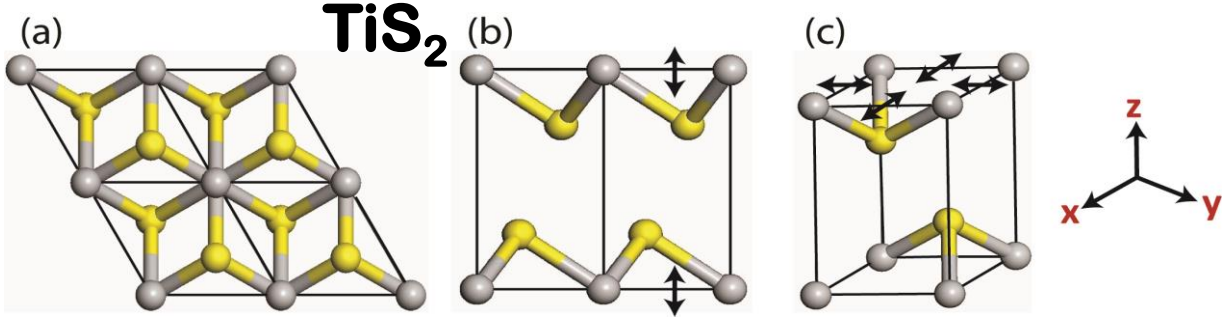
Novel 2D materials for photonics



Rossi, D.; Camacho-Forero, L. E.; Ramos-Sánchez, G.; Han, J. H.; Cheon, J.; Balbuena, P.; Son, D. H., *J. Phys. Chem. C* **2015**, *119* (13), 7436-7442

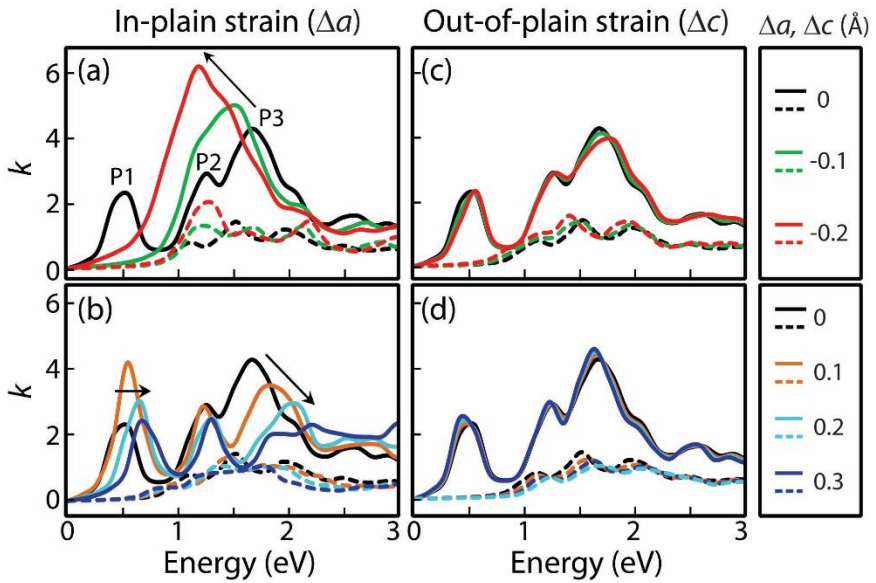
Accomplished through combined experimental & computational studies in high performance computers!!!

TiS_2



Calculated band structure elucidate optical transitions

Software: VASP;
Hardware: ADA



Imaginary part of refractive index (*k*) under varying degrees of lattice strain

Calculation shows effect of quantum confinement on optical properties

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Acknowledgements

Collaborators:
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Prof. Partha Mukherjee (TAMU)
Prof. Dong Hee Son (TAMU)
Prof. Hong-Cai Zhou (TAMU)
Prof. Vilas Pol (Purdue U)
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)

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Honda Research Institute
National Science Foundation
Qatar National Research Foundation

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