Introduction to Computational Materials Science

Instructor: Fernando A. Soto, PhD
Postdoctoral Research Associate, Chemical Engineering Department
Texas A&M University

Course Outcomes:
At the end of the lecture the students will be able to:
- Get a good understanding of different modeling techniques including density functional theory and *ab-initio* Molecular Dynamics
- Identify and apply different computational techniques on a variety of nanosystems
- Compute calculations combining the outputs of several simulations

Topics
1. Examples of Density Functional Theory in Action
2. Introduction to Density Functional Theory
3. VASP Tutorial
a. Pt atom
b. Pt bulk
c. Pt (111) surface
d. Pt (111) surface-O adsorption
4. Introduction to *ab-initio* Molecular Dynamics

CV

Instructor: Fernando A. Soto, PhD
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Fernando hold a M.Sc. and a Ph.D. in Engineering (Micro and Nanoscale Systems) from the Louisiana Tech University. He has a vast research experience as Postdoctoral research associate, Visiting scholar and Graduate Research Assistant.

The teaching and mentoring experience:

Shell-supported Northern Louisiana Regional Collaborative for Excellence in Science and Mathematics Teaching 2013

- Trained teachers from small rural and city schools around Louisiana Tech's region on computational chemistry concepts

• **Guest Lecturer "Computational Chemistry" during Engineering Science Day events at Louisiana Tech University, 2010-2014**

• **Nanosystems Modeling Course, Spring Quarter 2011-2014**

- Assisted with the syllabus design and planning of lessons
- Assisted with the evaluation and grade assignment of projects
- Regular Guest-lecturer and lectures on molecular dynamics, statistical mechanics, density functional theory to senior year chemical engineering students and graduate nanosystems engineering students

• Engineering Economics Course, Spring Quarter 2008

- Evaluated student's performance of cost analysis project
- Assisted with the evaluation and grade assignment of projects
- Conducted tutorial sessions on topics such as cash flow analysis

• **Thermodynamics Course, Spring Quarter 2020 at TAMU**

- Conducted tutorial session on solution thermodynamics

Areas of Interest

•Electrochemical Energy Storage • Hydrogen Energy Storage • Sustainable Concrete Engineering • Catalysis • Electrocatalysis • Corrosion Science • Additive Manufacturing • Optoelectronics • Machine Learning • Semiconductors • Hydrometallurgy • Neuromorphic Computing • Multi-functional Materials

Relevant Awards

• • School of Materials Science Engineering (MSEN) Postdoctoral Best Paper Award 2017

"Tuning the Solid Electrolyte Interphase for Selective Li- and Na-ion Storage in Hard Carbon" published in *Advanced Materials*

Texas A&M University, College Station TX

- • School of Materials Science Engineering (MSEN) Postdoctoral Best Paper Award 2016

“Formation and Growth Mechanisms of Solid-Electrolyte Interphase Layers in Rechargeable Batteries” published in *Chemistry of Materials*
Texas A&M University, College Station TX

- • **2nd Place, Texas A&M University Postdoctoral Research Symposium Poster Competition 2017**

“Understanding and Controlling the Li-Ion Transport through a Graphene Oxide Coating for Dendrite Suppression”
Texas A&M University, College Station TX

- • **2nd Place, NSF EPSCoR LA-SiGMA Poster Competition 2013**

"On the Road for Clean Energy: Computational Study of Catalysts for Fischer-Tropsch Reactions"