Quantum Mechanical Simulations and Their Applications to Clean Energy.

Jose L. Mendoza-Cortes
Courtesy Professor, Florida State University

In the first part of the talk we will discuss some of the fundamental problems related to clean energy and a way to solve them. We will discuss some of the efforts we have been making for this dream of carbon neutral energy to become a reality. We will present some accomplishments in the areas of energy storage, catalysis and photovoltaics, as well as carbon capture. We will explain how theoretical and simulation efforts are aiding in this enterprise. More specifically, we will discuss the conversion of water to fuel from the sun and a carbon neutral cycle using sunlight. These are examples where atomistic simulations are being used to predict new materials and molecules, as well as to design new catalysts and photovoltaics for a greener future.

In the second part of the talk, I will discuss new methods and new theoretical frameworks that would be useful in the new paradigm that the 21st century brings. I will talk more specifically about Quantum Electrodynamics for Chemistry, Reactive Force Fields, and Multiscale Simulations. These new theoretical and simulation methods will be useful in other applications such as Energy Storage, Materials Design, Biomaterials, Catalysis, Electrochemistry, Crystallization Mechanisms, and Processes.

Bio-sketch

Postdoctoral Researcher, UC Berkeley & Berkeley National, 2014
Staff Scientist, California Institute of Technology & Joint Center for Artificial Photosynthesis, 2013
Ph.D., California Institute of Technology, 2012
M.S., California Institute of Technology, 2010
B.S., Tec de Monterrey (ITESM), 2008.
University of California, Los Angeles (UCLA), 2006-2008