Consiglio Nazionale delle Ricerche
Istituto di Chimica dei Composti OrganoMetallici

22 Maggio 2019
alle ore 11.00

presso l' AULA 27 dell'Edificio A
Area della Ricerca CNR
Via Giuseppe Moruzzi, 1 Pisa (PI)

il Dr. WILLIAM A. GODDARD
California Institute of Technology
Pasadena, CA, USA

terrà il seguente seminario:

" New Quantum Mechanics based methods for Multiscale simulations with applications to reaction mechanisms for Electrocatalysis"

Dr. Alessandro Fortunelli
Primo Ricercatore

Dr. Francesco Vizza
Direttore ICCOM

Short Abstract:

Advances in theory and methods of quantum mechanics are making it practical for first principles (de novo) predictions of the mechanisms of complex electrocatalytic reactions.
We will highlight some recent advances in such methodologies including:

- Grand canonical QM calculations of electrochemical catalysis at constant potential (instead of constant numbers of electrons)
- QM Metadynamics calculations of free energies of electrocatalysis at operational temperature and potential
- New generation reactive force fields with polarization and universal nonbond interactions
- Machine learning to identify active sites on NP and NW
- Hybrid QM-ReaxPQ dual embedding for battery and electrocatalysis applications

which we will illustrate with recent applications to the reaction mechanisms for electrocatalysis including:

- The CO2 reduction reaction on Au ,Ag, Cu and alloys: (100), (111), and Nanoparticles
- The oxygen evolution on IrO2 and NiOOH doped with Fe and other metals
- The oxygen reduction reaction (ORR) on Pt (111) vs. dealloyed NiPt nanowires
- The hydrogent evolution reaction for (XNH3)PbI3 photocatalysts and for MoS2
- Application of reactive force fields and machine learning to electrocatalysis on nanoparticles (NP) and nanowires (NW)
- Operando vibrational frequencies and XPS shifts for the Electrode-Electrode Interface

Biographic sketch:

Goddard Brief CV

Goddard received his BS Engineering from UCLA and his PhD in Engineering Science with a minor in Physics in Oct. 1964. He has been on the Caltech faculty since Nov. 1964 where he is the Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics and Director of the Materials and Process Simulation Center (MSC).

Goddard has been a pioneer in developing methods for quantum mechanics (QM), force fields (FF), reactive dynamics (ReaxFF RD), electron dynamics (eFF), molecular dynamics (MD), and Monte Carlo (MC) predictions on chemical, catalytic, and biochemical materials systems

He is actively involved in applying these methods to ceramics, semiconductors, superconductors, thermoelectrics, metal alloys, polymers, proteins, nuclei acids, Pharma ligands, nanotechnology, and energetic materials. Current foci include developing new electrocatalysts for water splitting (producing H_2 and O_2 from water), CO_2 reduction to organics, on the oxygen reduction reaction and development pf powerful methods for predicting the structures of membrane bound proteins and the binding sites of agonists and antagonists.

He was elected to the National Academy of Science (1984, age 47) and to the International Academy of Quantum Molecular Science (1986).

He is a Fellow of the American Physical Society (1988), the American Association for the Advancement of Science (1990), the Royal Society Chemistry (2008), and the American Academy of Arts and Sciences (2010).

He was Awarded Honoris Causa Philosophia Doctorem, Chemistry, Uppsala U., Sweden, January 2004.

He was the winner of the American Chemical Society Award for Computers in Chemistry (1988), the Feynman Prize for Nanotechnology Theory (1999), the Richard Chase Tolman Prize from the Southern California Section ACS (2000), the American Chemical Society Award for Theoretical Chemistry (2007), the NASA Space Sciences Award for Space Shuttle Sensor (2009), the NASA Space Sciences Award for polymer films (2012), and the Distinguished Scientific Achievement Catalysis Award from the 7th World Congress Oxidation Catalysis (2013).

He was named ISI Highly Cited Chemist for 1981-2001, 2014, 2015, 2016 and the Clarivate Analytics Highly Cited Researcher for 2018. His H-index is currently 134.

https://en.wikipedia.org/wiki/William_Andrew_Goddard_III