Consiglio Nazionale delle Ricerche
Istituto di Chimica dei Composti OrganoMetallici

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alle ore 15.00

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:

" Predicted Iron alloy catalysts with dramatically improved rates for Haber Bosch Synthesis of NH_3 using *in silico* QM based hierarchical high-throughput catalysts screening"

Dr. Alessandro Fortunelli
Primo Ricercatore

Dr. Francesco Vizza
Direttore ICCOM

Short Abstract:

The Haber-Bosch (HB) industrial process for synthesis of ammonia (NH_3) from hydrogen and nitrogen produces the millions of tons of ammonia gas annually needed to produce the nitrates for fertilizers required to feed the earth's growing populations. Despite 100 years of empirical optimization, HB uses ~ 2% of the world's supply of energy while operating at extreme conditions (200 atm and >500 °C), requiring huge capital investments. To provide guidelines for dramatically accelerating the rates to allow much less extreme conditions, we used quantum mechanics based *in silico* hierarchical high-throughput catalysts screening (HHTCS) to predict new Fe-based alloys.

As the basis for these predictions, we used QM to predict the 26 surface configurations of reaction intermediates important for the conditions (400 °C and 20 atm) used in the single crystal studies by Somorjai and predicted the free energy based kinetic rates for the most important 13 rate processes. Then we solved the kinetic Monte Carlo rates for 30 to 45 minutes of steady state reactions to obtain the turn over frequencies (TOF), which are in excellent agreement with single crystal experiments.

Then we carried out *in silico* HHTCS to predict new ternary alloys selected to place one dopant at the surface while the other is subsurface. This leads to dramatically increased rates (~100) for HB conditions, allowing much lower pressures to achieve the same TOF.

This illustrates a new strategy that can be used to optimize catalyst performance for complex reactions involving 10 to 20 potential rate determining steps, where the simple Sabatier-principle-based volcano relationships in terms of a single controlling parameter no longer apply.

Funding: DOE-EERE-AMO

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