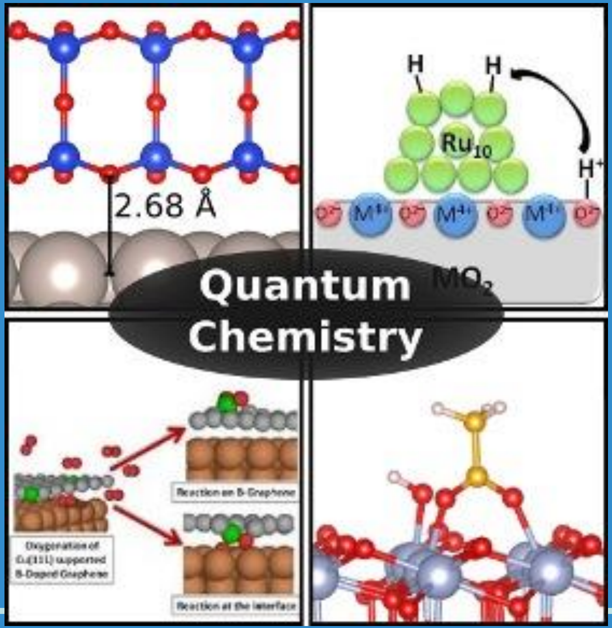
Theory of Inorganic Materials for Energy and Environment

Quantum Chemistry Laboratory
Dipartimento di Scienza dei Materiali
Università Milano-Bicocca
https://qclab.mater.unimib.it/



THE GROUP AT UNIMIB

THE GROUP AT UNIMIB

Gianfranco Pacchioni

Full Professor, Editor-in-chief Journal of Physics: Condensed Matter

Former vice-rector, former Director of the Department, former president DCTC, Accademia Nazionale dei Lincei, etc

Livia Giordano

Associate Professor

Sergio Tosoni

Associate Professor

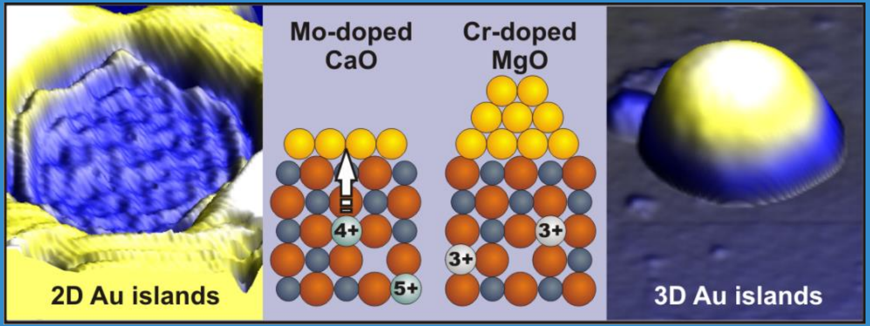
Giovanni Di Liberto

Assistant Professor

Quantum Chemistry Laboratory
THREE MAIN RESEARCH LINES

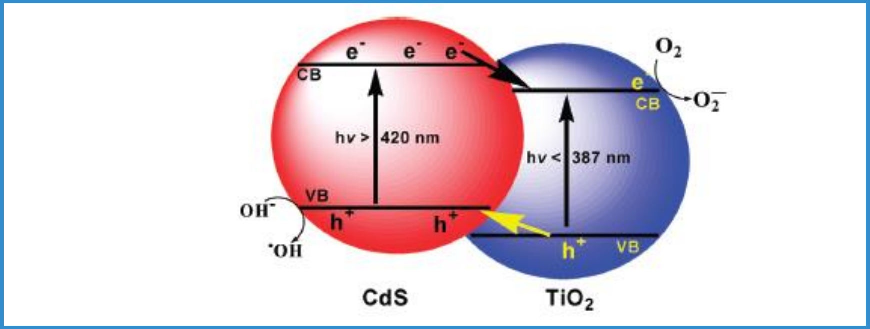
Nanostructured oxides and thin films

Microelectronics, spintronics, catalysis

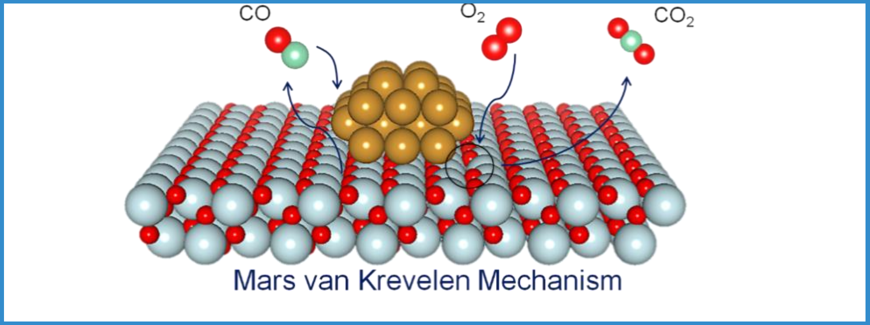


Semiconducting materials in photocatalysis

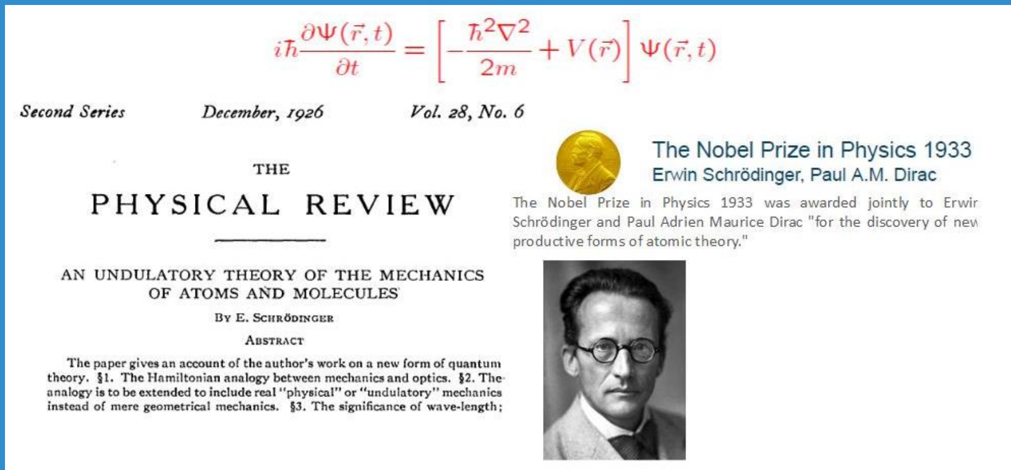
Band gap engineering

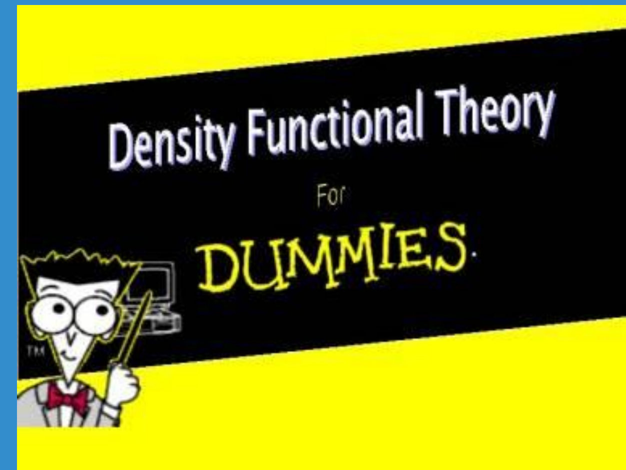


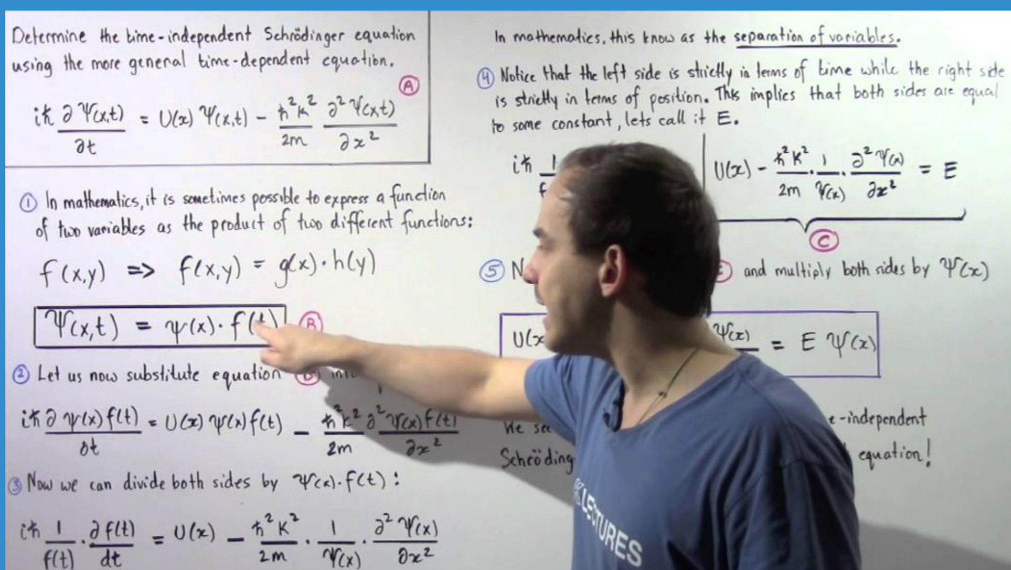
Nanoparticles in catalysis for water splitting, fuel cell, CO_2 valorization



PRACTICAL SOLUTION OF THE SCHRÖDINGER EQUATION: DFT

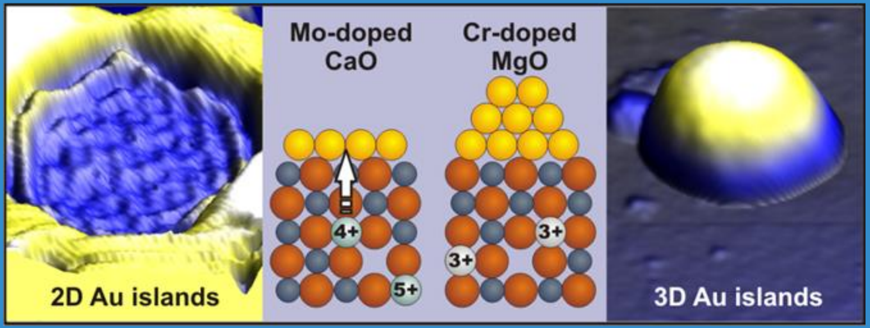






Nanostructured oxides and thin films

Microelectronics, spintronics, catalysis

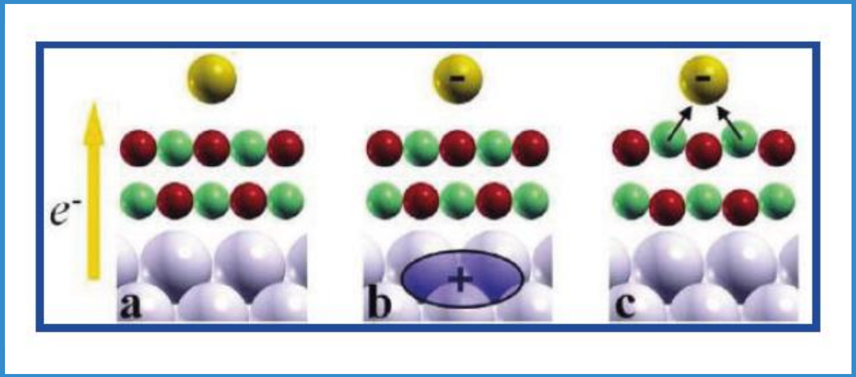


ACCOUNTS
of chemical research

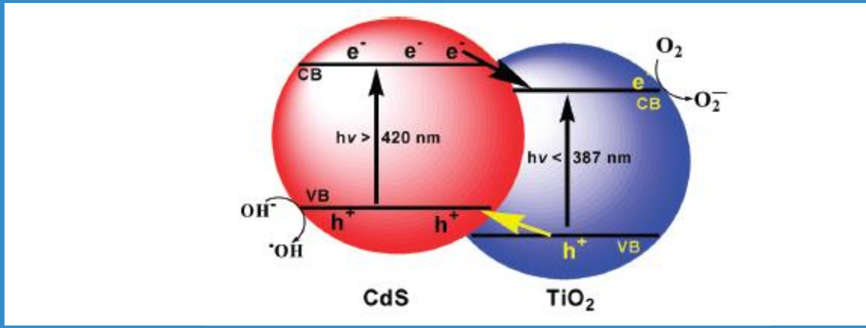
Oxide Films at the Nanoscale: New Structures, New Functions, and New Materials

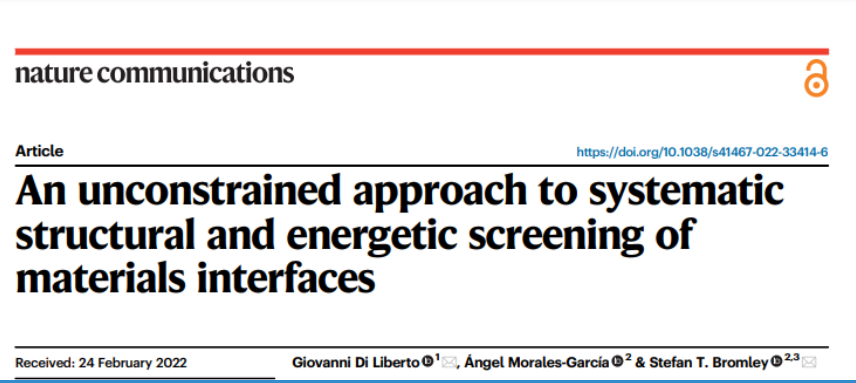
LIVIA GIORDANO AND GIANFRANCO PACCHIONI*

Dipartimento di Scienza dei Materiali, Università Milano Bicocca, via R. Cozzi 53, 53-20125 Milano, Italy



Semiconducting materials in photocatalysis




nature communications

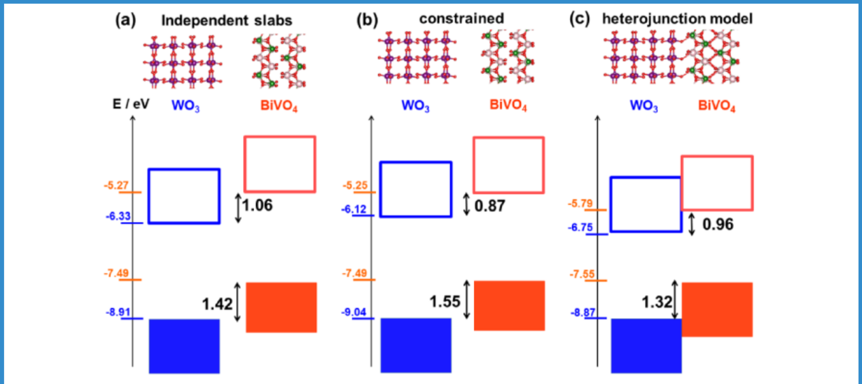
Article

https://doi.org/10.1038/s41467-022-33414-6

An unconstrained approach to systematic structural and energetic screening of materials interfaces

Received: 24 February 2022

Giovanni Di Liberto[1], Ángel Morales-García[2] & Stefan T. Bromley[2,3]



Material design for electrocatalysis

nature catalysis | ARTICLES
https://doi.org/10.1038/s41929-021-00668-0
Check for updates

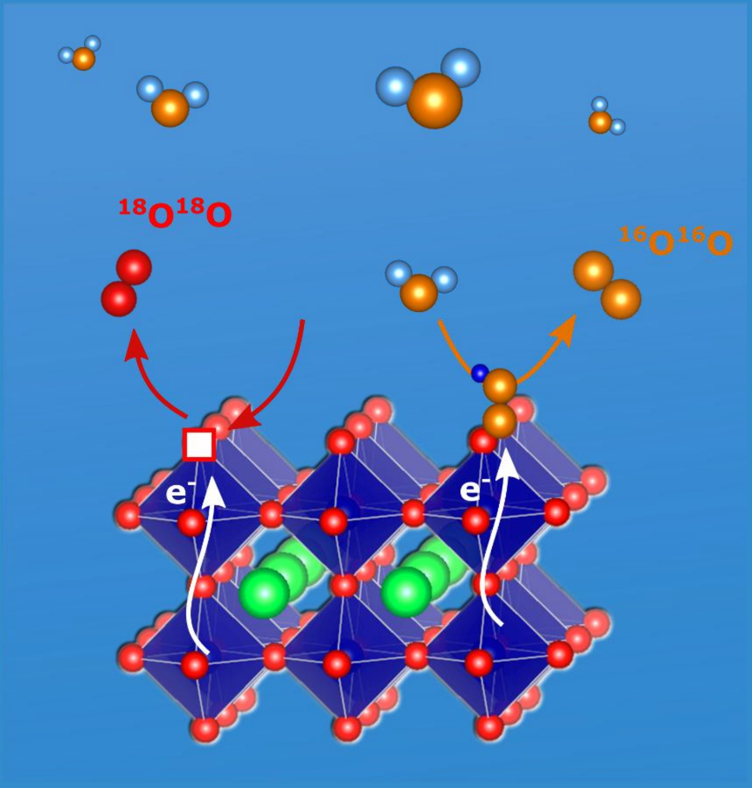
Enhancing oxygen reduction electrocatalysis by tuning interfacial hydrogen bonds

nature chemistry | ARTICLES
PUBLISHED ONLINE: 9 JANUARY 2017 | DOI: 10.1038/NCHEM.2695

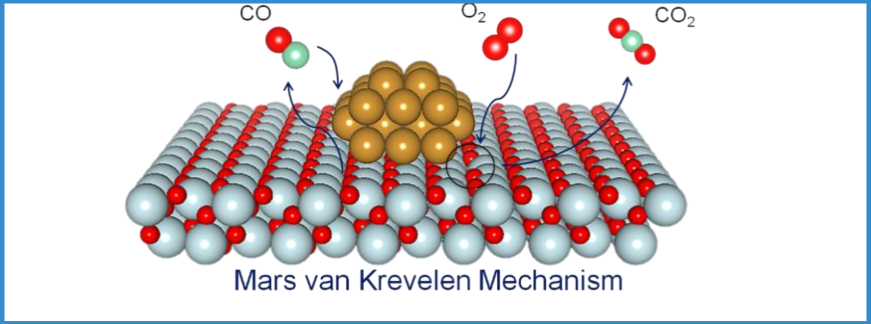
Activating lattice oxygen redox reactions in metal oxides to catalyse oxygen evolution

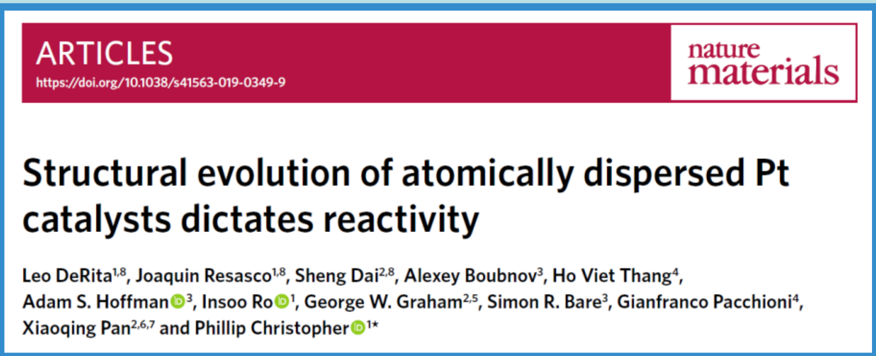
nature materials | ARTICLES
https://doi.org/10.1038/s41563-022-01199-0
Check for updates

Tunable metal hydroxide–organic frameworks for catalysing oxygen evolution



Nanoparticles in catalysis for water splitting, fuel cell, CO_2 valorization

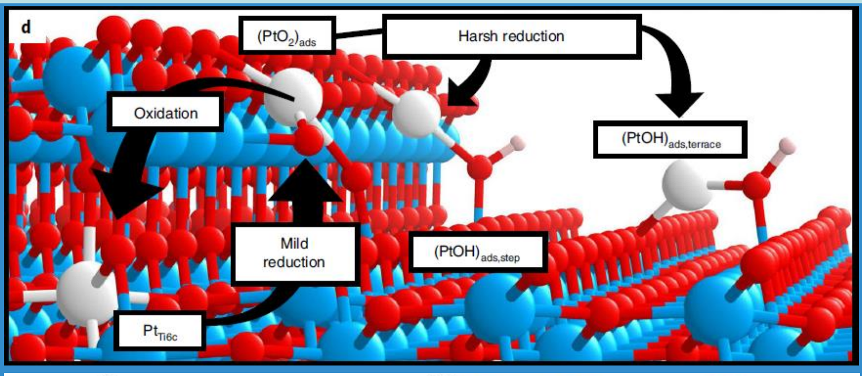


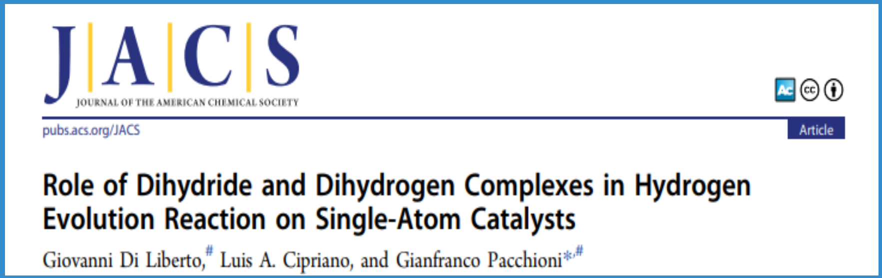


ARTICLES
https://doi.org/10.1038/s41563-019-0349-9
nature materials

Structural evolution of atomically dispersed Pt catalysts dictates reactivity

Leo DeRita[1,8], Joaquin Resasco[1,8], Sheng Dai[2,8], Alexey Boubnov[3], Ho Viet Thang[4], Adam S. Hoffman[3], Insoo Ro[1], George W. Graham[2,5], Simon R. Bare[3], Gianfranco Pacchioni[4], Xiaoqing Pan[2,6,7] and Phillip Christopher[1]*

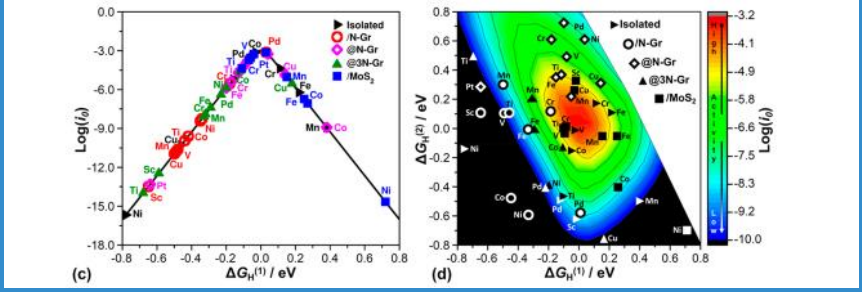


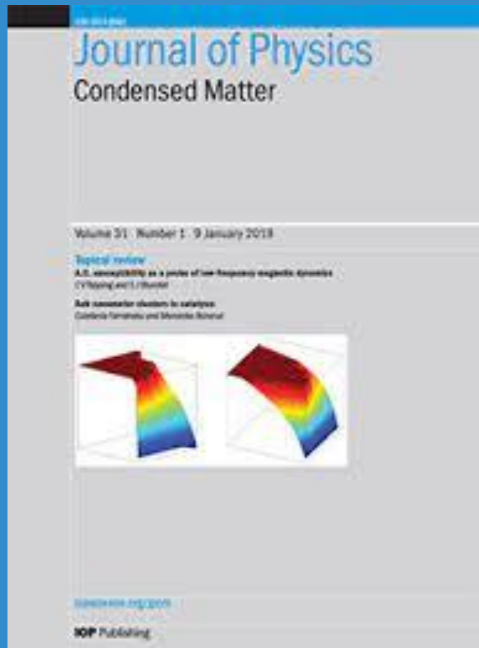


JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
pubs.acs.org/JACS
Article

Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts

Giovanni Di Liberto,[#] Luis A. Cipriano, and Gianfranco Pacchioni*[,#]





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Editor-in-Chief

Gianfranco Pacchioni Universitá degli Studi di Milano-Bicocca, Italy

INTERNATIONAL COLLABORATIONS AND PROJECTS

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Univ. Leuven

Recent projects:

Cariplo Foundation 2022-2025 – New Materials for circular economy

MIUR PRIN 2016-2019 – New materials for CO_2 and H_2 cataysis

MIUR FIRB 2011-2016 – Nanostructured oxides

Cariplo Foundation 2014-2017 – Oxides photocatalysis

CASCATBEL – FP7 2014-2018 – Oxide catalysts for biofuels

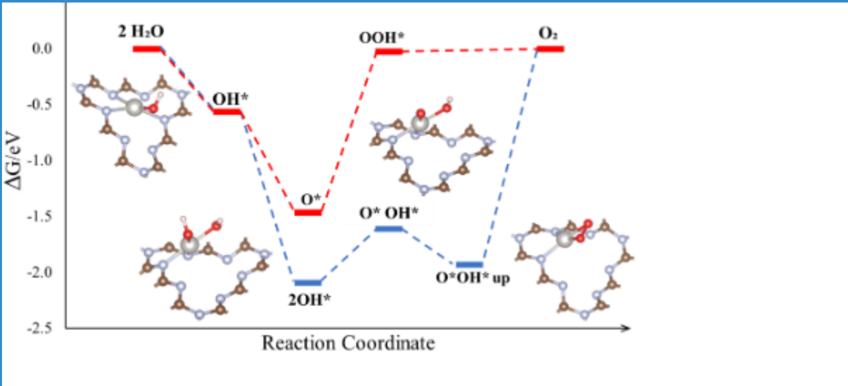
CATSENSE – FP7 2014-2018 – Metal clusters on oxides

COST CM1104 – 2013-2017 - Reducible oxides

Some Examples?

Bachelor Thesis

Water Splitting on a Pt_1/C_3N_4 Single Atom Catalyst: a modeling approach



New chemical insights

On-going reactions

Structure-property relantionships