

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



Giovanni Di Liberto– Dept. Materials Science – Univ. Milano Bicocca

Quantum Chemistry Laboratory

THREE MAIN RESEARCH LINES

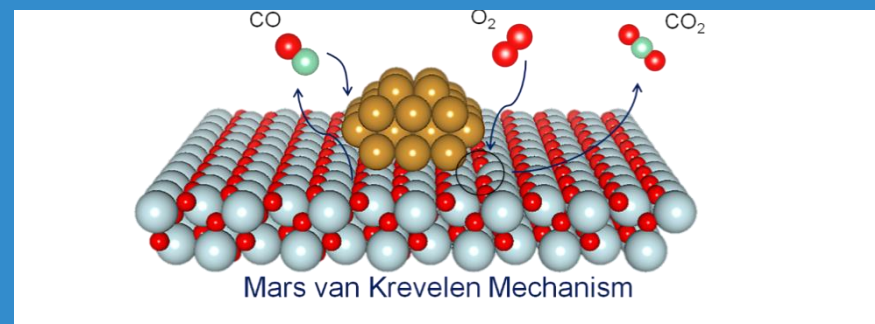
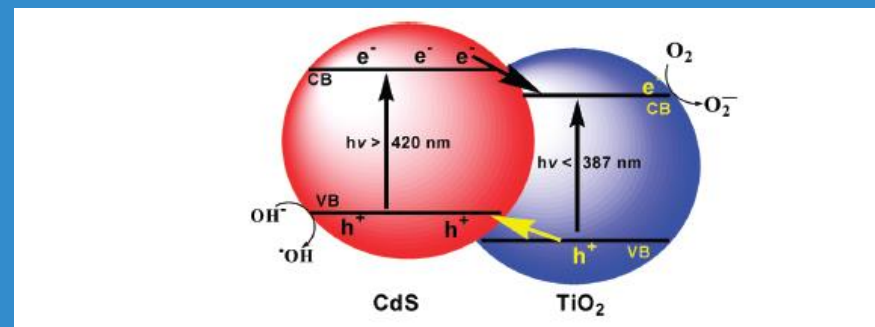
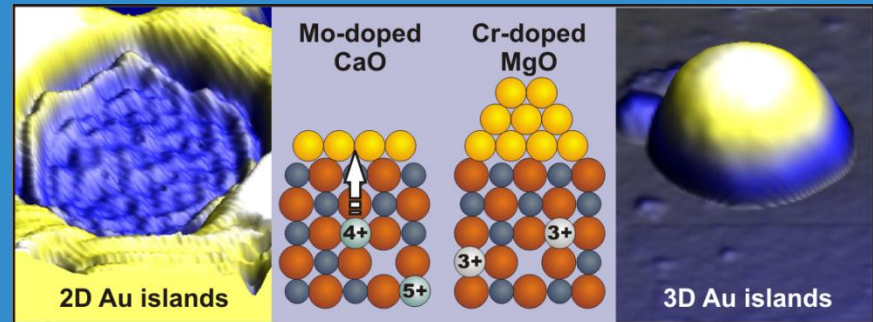
Nanostructured oxides and thin films

Microelectronics, spintronics, catalysis

Semiconducting materials in photocatalysis

Band gap engineering

Nanoparticles in catalysis for water splitting, fuel cell, CO₂ valorization



PRACTICAL SOLUTION OF THE SCHRÖDINGER EQUATION: DFT

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) \right] \Psi(\vec{r}, t)$$

Second Series December, 1926 Vol. 28, No. 6

THE PHYSICAL REVIEW

AN UNDULATORY THEORY OF THE MECHANICS OF ATOMS AND MOLECULES

By E. SCHRÖDINGER

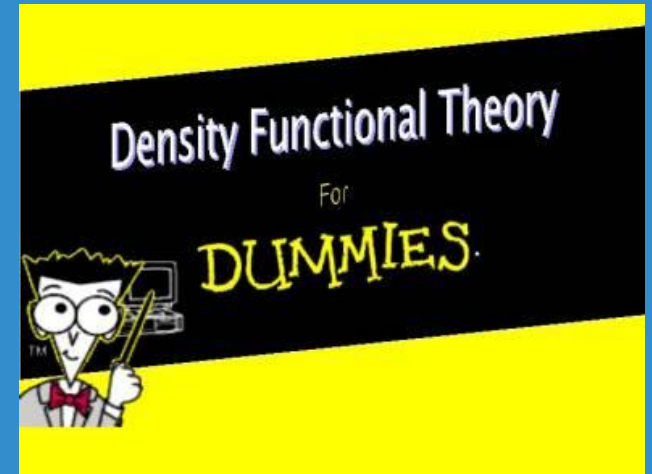
ABSTRACT

The paper gives an account of the author's work on a new form of quantum theory. §1. The Hamiltonian analogy between mechanics and optics. §2. The analogy is to be extended to include real "physical" or "undulatory" mechanics instead of mere geometrical mechanics. §3. The significance of wave-length;



The Nobel Prize in Physics 1933
Erwin Schrödinger, Paul A.M. Dirac

The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory."



Determine the time-independent Schrödinger equation using the more general time-dependent equation.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = U(x) \Psi(x,t) - \frac{\hbar^2 k^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} \quad (A)$$

① In mathematics, it is sometimes possible to express a function of two variables as the product of two different functions:

$$f(x,y) \Rightarrow f(x,y) = g(x) \cdot h(y)$$

$$\Psi(x,t) = \psi(x) \cdot f(t) \quad (A)$$

② Let us now substitute equation (A) into (1).

$$i\hbar \frac{\partial \psi(x)f(t)}{\partial t} = U(x) \psi(x)f(t) - \frac{\hbar^2 k^2}{2m} \frac{\partial^2 \psi(x)f(t)}{\partial x^2}$$

③ Now we can divide both sides by $\psi(x) \cdot f(t)$:

$$i\hbar \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = U(x) - \frac{\hbar^2 k^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2}$$

In mathematics, this is known as the separation of variables.

④ Notice that the left side is strictly in terms of time while the right side is strictly in terms of position. This implies that both sides are equal to some constant, let's call it E.

$$i\hbar \frac{1}{f} \frac{\partial f}{\partial t} = U(x) - \frac{\hbar^2 k^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} = E \quad (C)$$

⑤ Now we can separate the variables by multiplying both sides by $\psi(x)$.

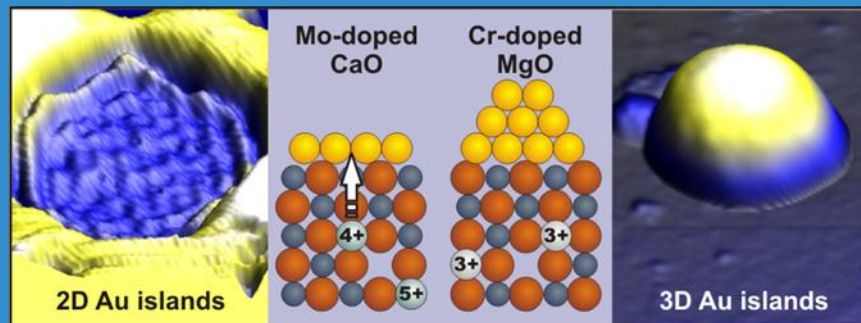
$$U(x) \psi(x) = E \psi(x)$$

We see that the left side is strictly in terms of position and the right side is strictly in terms of time. This is the time-independent Schrödinger equation!



Nanostructured oxides and thin films

Microelectronics, spintronics, catalysis

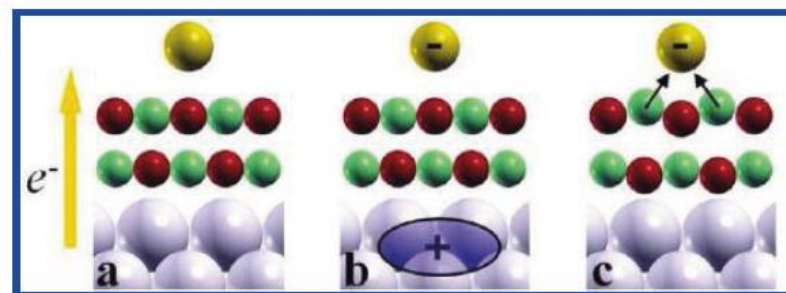


ACCOUNTS
of chemical research

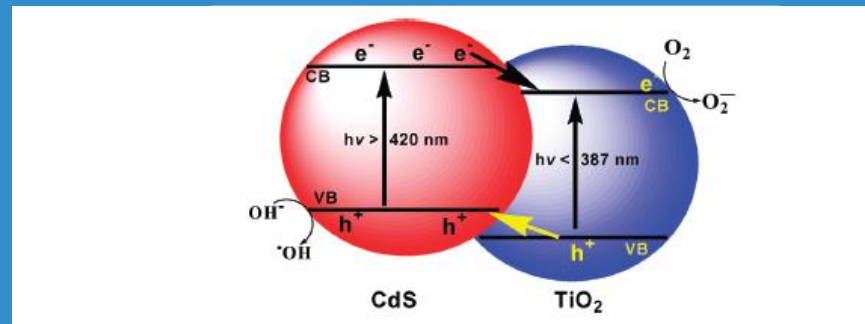
Oxide Films at the Nanoscale: New Structures, New Functions, and New Materials

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



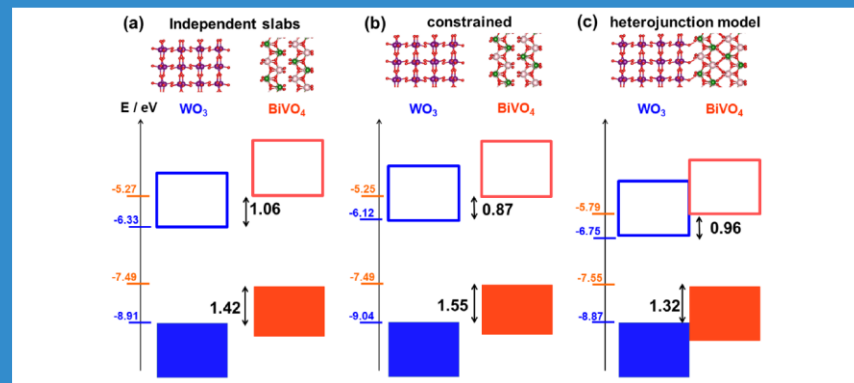
Article

<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 Liberto¹, Ángel Morales-García² & Stefan T. Bromley^{2,3}



Material design for electrocatalysis

nature
catalysis

ARTICLES

<https://doi.org/10.1038/s41929-021-00668-0>



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

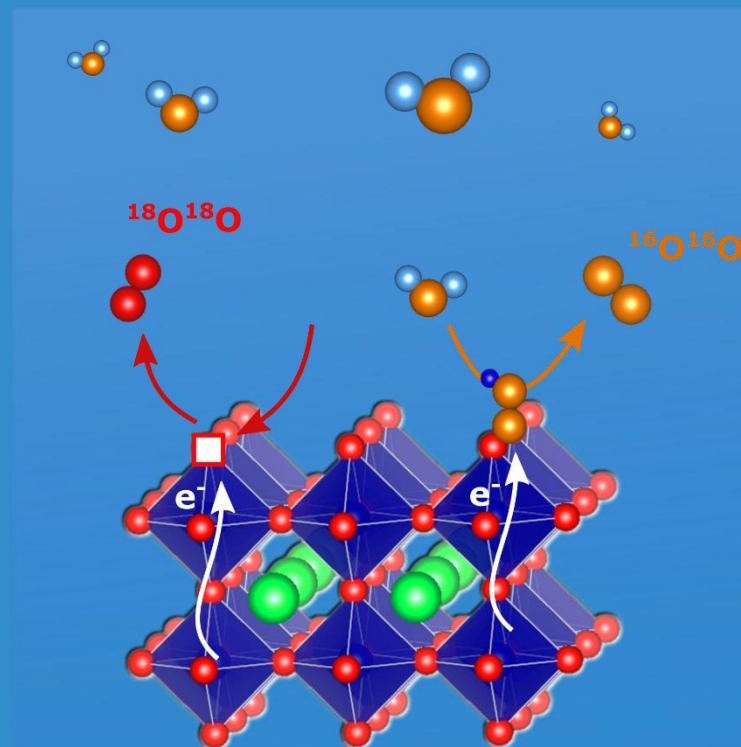
nature
materials

ARTICLES

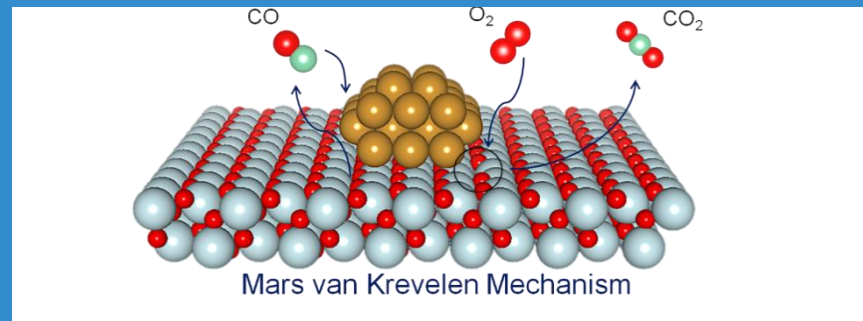
<https://doi.org/10.1038/s41563-022-01199-0>



Tunable metal hydroxide–organic frameworks for catalysing oxygen evolution



Nanoparticles in catalysis for water splitting, fuel cell, CO₂ 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 Boubnov³, Ho Viet Thang⁴, Adam S. Hoffman³, Insoo Ro¹, George W. Graham^{2,5}, Simon R. Bare³, Gianfranco Pacchioni⁴, Xiaoqing Pan^{2,6,7} and Phillip Christopher^{1*}

JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

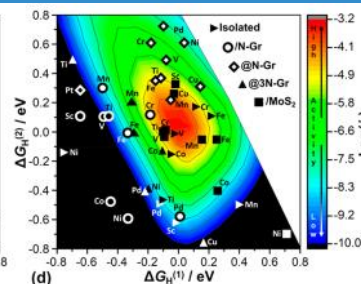
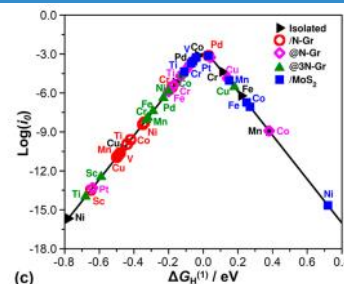
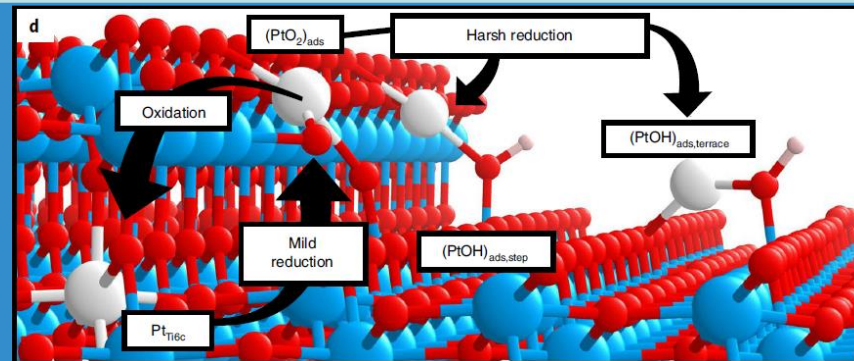
pubs.acs.org/JACS

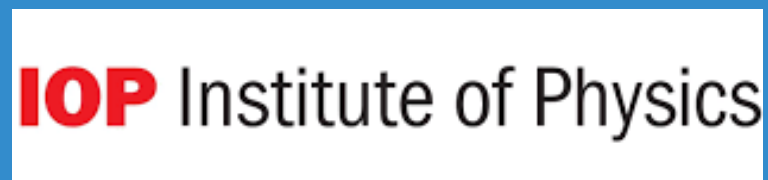
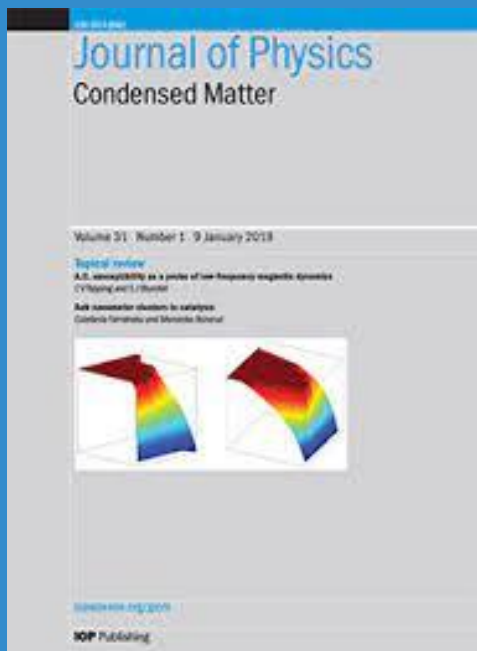




Article

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

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





IOPscience  Journals ▾ Books Publishing Support  Login ▾

Journal of Physics: Condensed Matter

Editorial Board

Journal of Physics: Condensed Matter is led by an Executive Board comprising of the Editor-in-Chief and ten Section Editors, who oversee the wider Editorial Board.

Editor-in-Chief

[Gianfranco Pacchioni](#) Università degli Studi di Milano-Bicocca, Italy



INTERNATIONAL COLLABORATIONS AND PROJECTS



HJ Freund

Fritz Haber MPI Berlin



N Nilius

B Lechner

Univ. Munich



P Christofer

U. S. Barbara



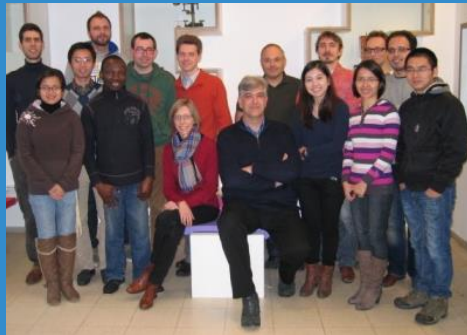
J Behm

Univ. Ulm



Y Shao-Horn

MIT



P. Lievens

Univ. Leuven

Recent projects:

Cariplo Foundation 2022-2025 – New Materials for circular economy

MIUR PRIN 2016-2019 – New materials for CO₂ and H₂ cataysis

MIUR FIRB 2011-2016 – Nanostructured oxides

Cariplo Foundation 2014-2017 – Oxides photocatalysis

CASCATBEL – FP7 2014-2018 – Oxide catalysts for biofuels

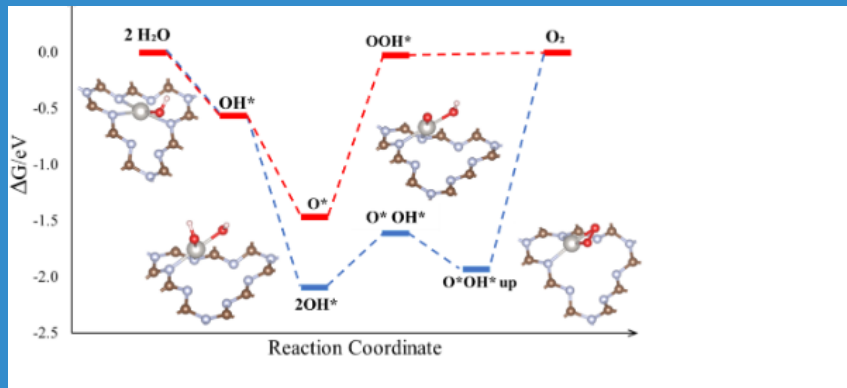
CATSENSE – FP7 2014-2018 – Metal clusters on oxides

COST CM1104 – 2013-2017 - Reducible oxides

Some Examples?

Bachelor Thesis

Water Splitting on a Pt₁/C₃N₄ Single Atom Catalyst: a modeling approach



New chemical insights

On-going reactions

Structure-property relationships