On the search of new lightweight materials for the automotive technology: a computational approach

Jimena A. Olmos-Asar

Departamento de Química Teórica y Computacional, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba – INFIQC, CONICET

FCQ
Facultad de
Ciencias Químicas

UNC

CONICET

INFIQC, FCQ, UNC

Marcelo Mariscal

PhD - Chemistry

2008 2012

Universitá degli Studi di Trieste

María Peressi

INFIQC, FCQ, UNC

Marcelo Mariscal

PhD - Chemistry | Postdoc

2008 2012 2013 2014

Universitá degli Studi di Trieste

María Peressi

UFABC

Adalberto Fazzio

INFIQC, FCQ, UNC

Marcelo Mariscal

PhD - Chemistry | Postdoc | ... | Postdoc

2008 2012 2013 2014 2015 2016 2017

Where do we work?

Departamento de Química Teórica y Computacional,
Facultad de Ciencias Químicas,
Universidad Nacional de Córdoba

Instituto de Investigaciones en Físico-Química de Córdoba, **CONICET**

Who are we?

Marcelo Mariscal
group leader

Fábio Negreiros Ribeiro
researcher

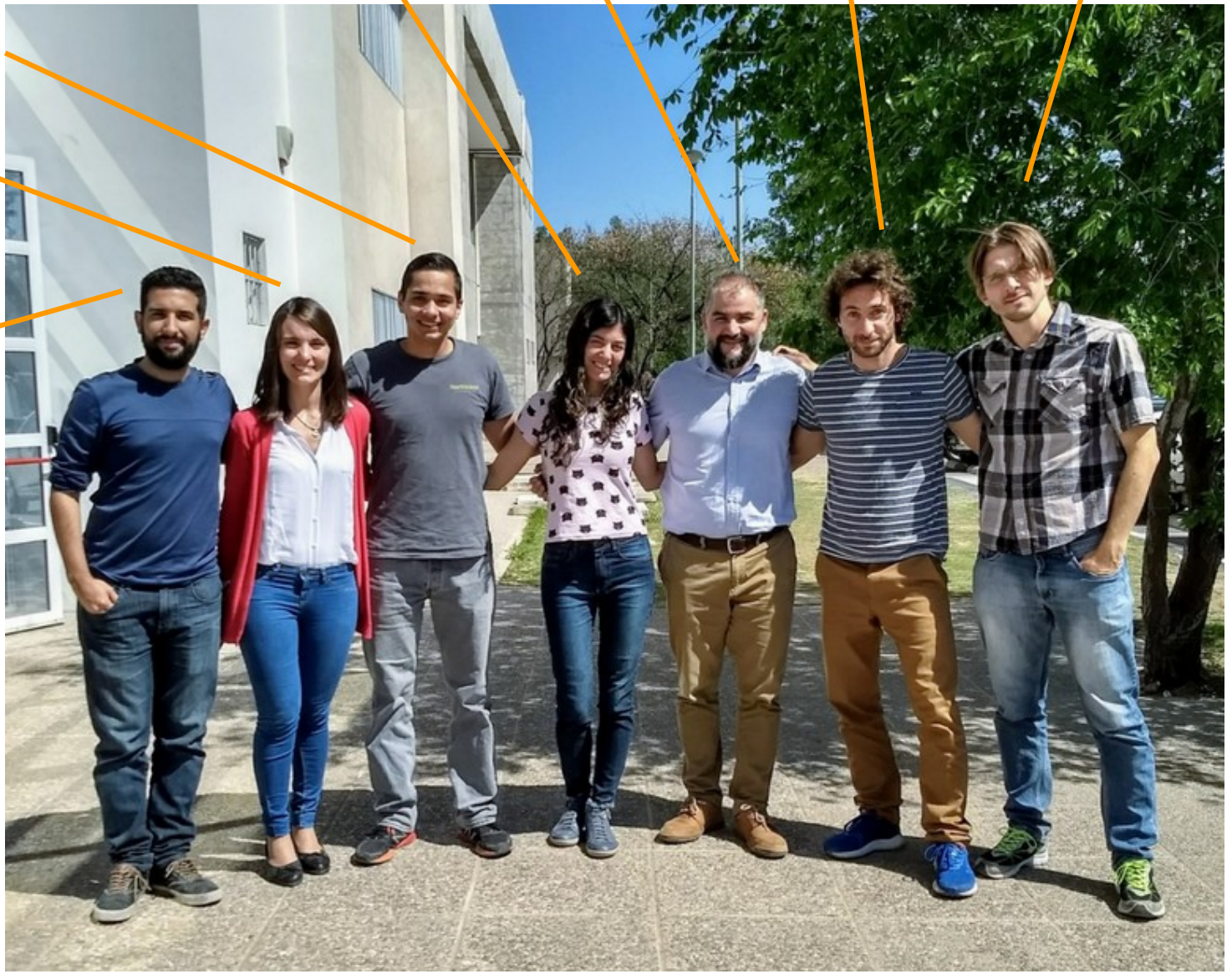
Jimena Olmos Asar
researcher

Germán Soldano
researcher

Juan de la Rosa Abad
PhD student

Paula Cappellari
postdoc

Juan Carlos Jiménez
PhD student



What do we research?

Development of classical potentials

Heterogeneous catalysis

2D materials and interfaces

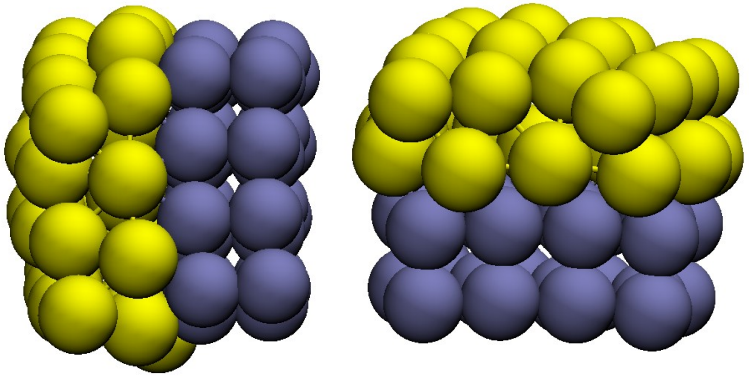
Oxides

Passivation of metal nanoparticles

Mechanical properties of nanosystems

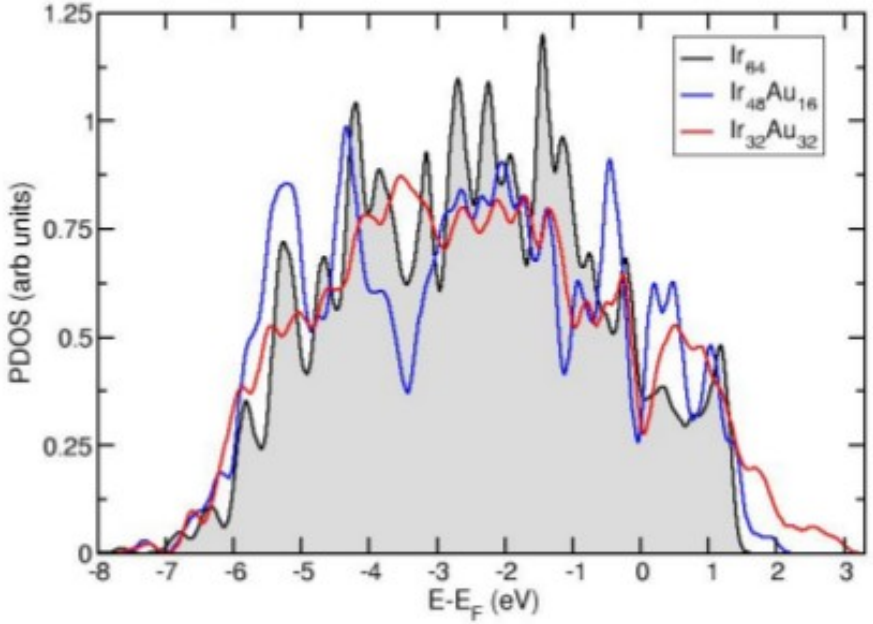
Global minimization techniques

IrAu Nanoalloys

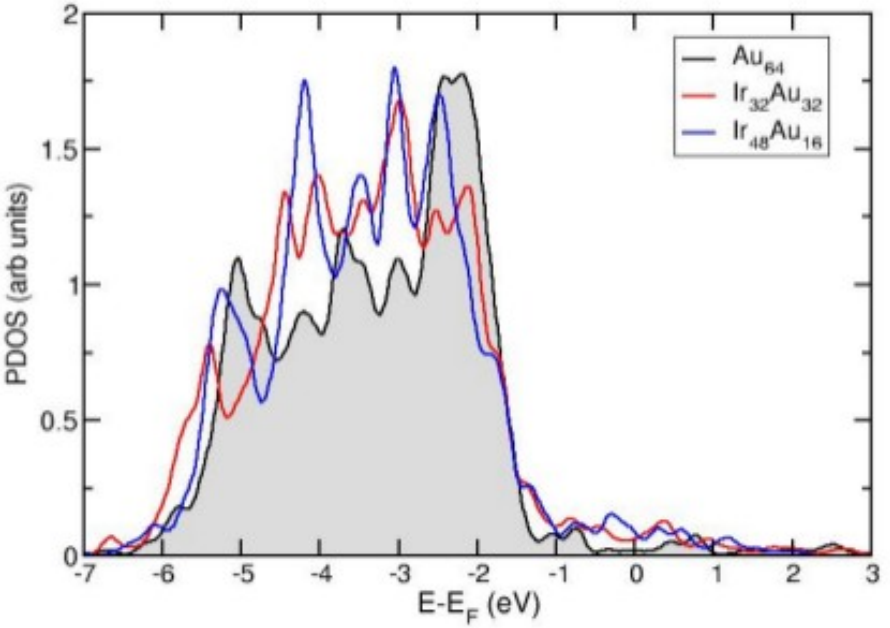


- Different Ir and Au environments
- Notable segregation tendency
- Au atoms increase the reactivity of Ir atoms

Ir d-orbital



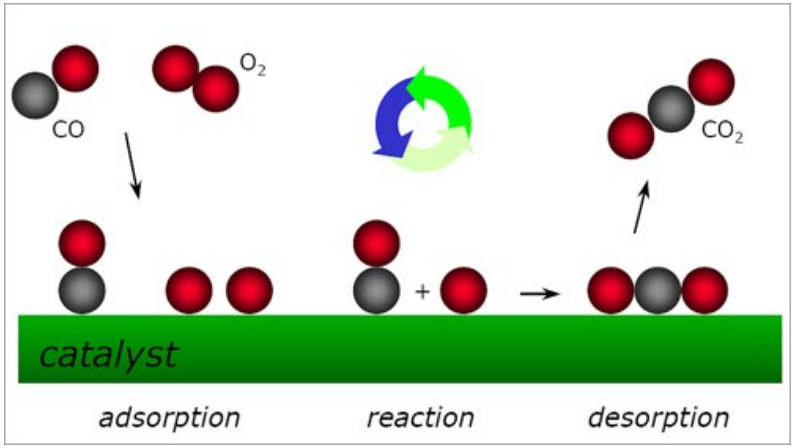
Au d-orbital



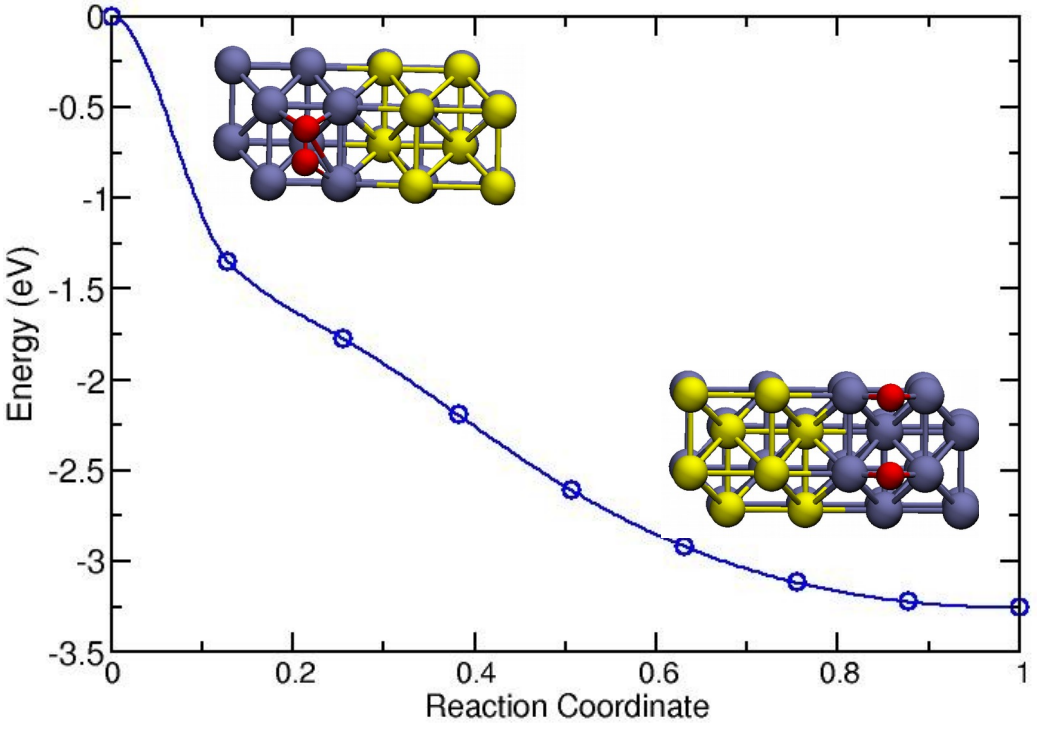
Cappellari P. S., Soldano G. J. and Mariscal, M. M., "A density functional study on the reactivity enhancement induced by gold in IrAu nanoalloys", RSC Adv., 8, 10450-10456, 2018.

CO Oxidation on Bimetallic Nanolloys

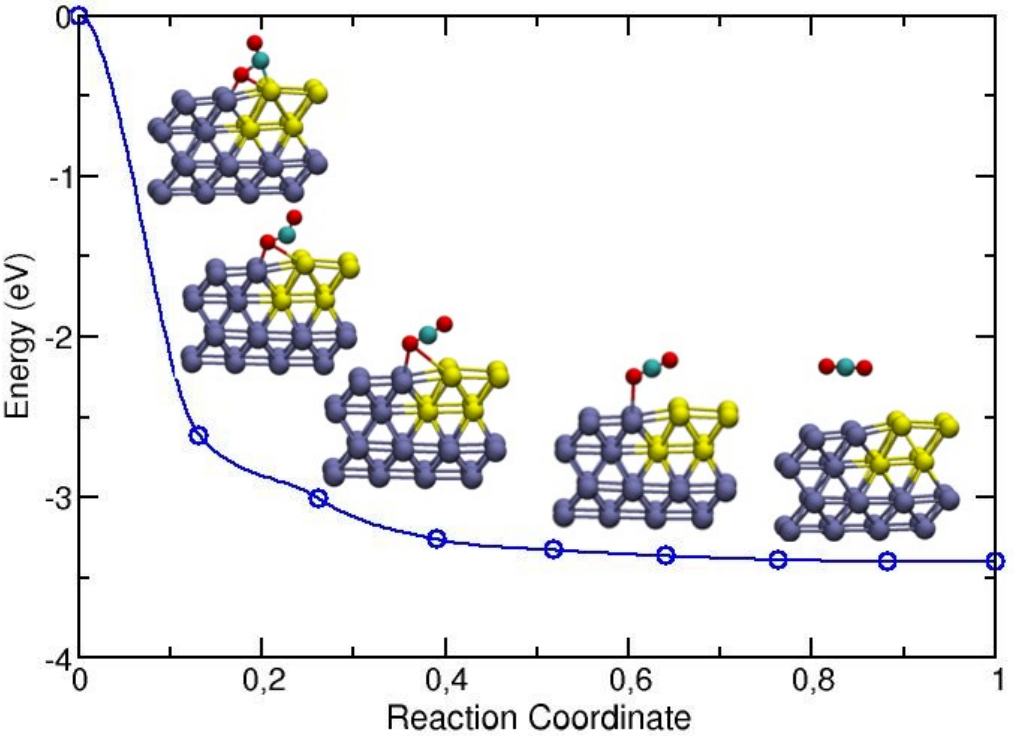
- O_2 dissociation favored on Ir region
- Spontaneous formation of CO_2 on Au and IrAu interface
- Low activation energy for O_{at} diffusion on Ir areas



O_2 Dissociation

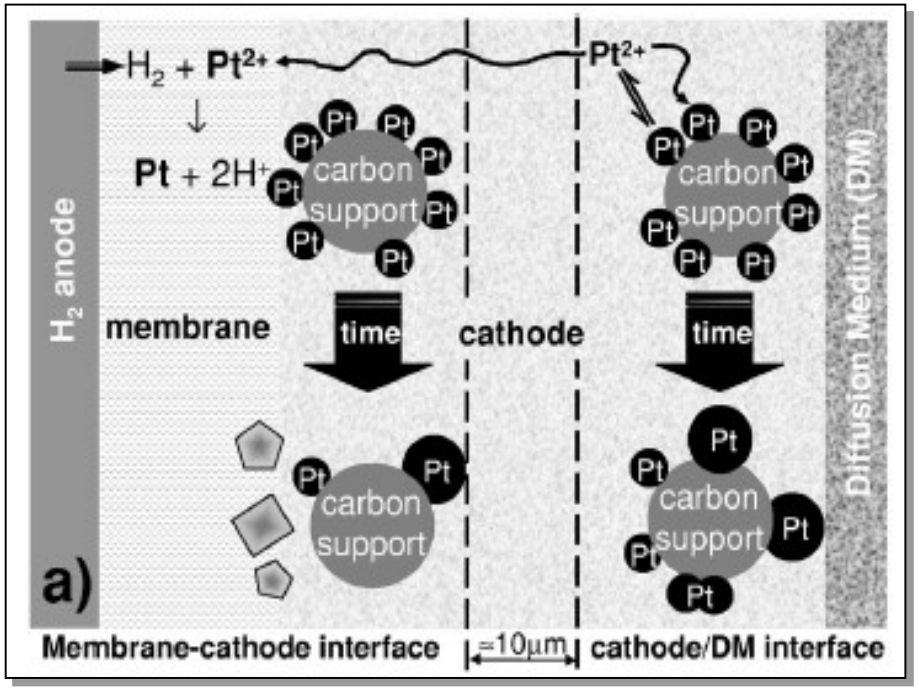


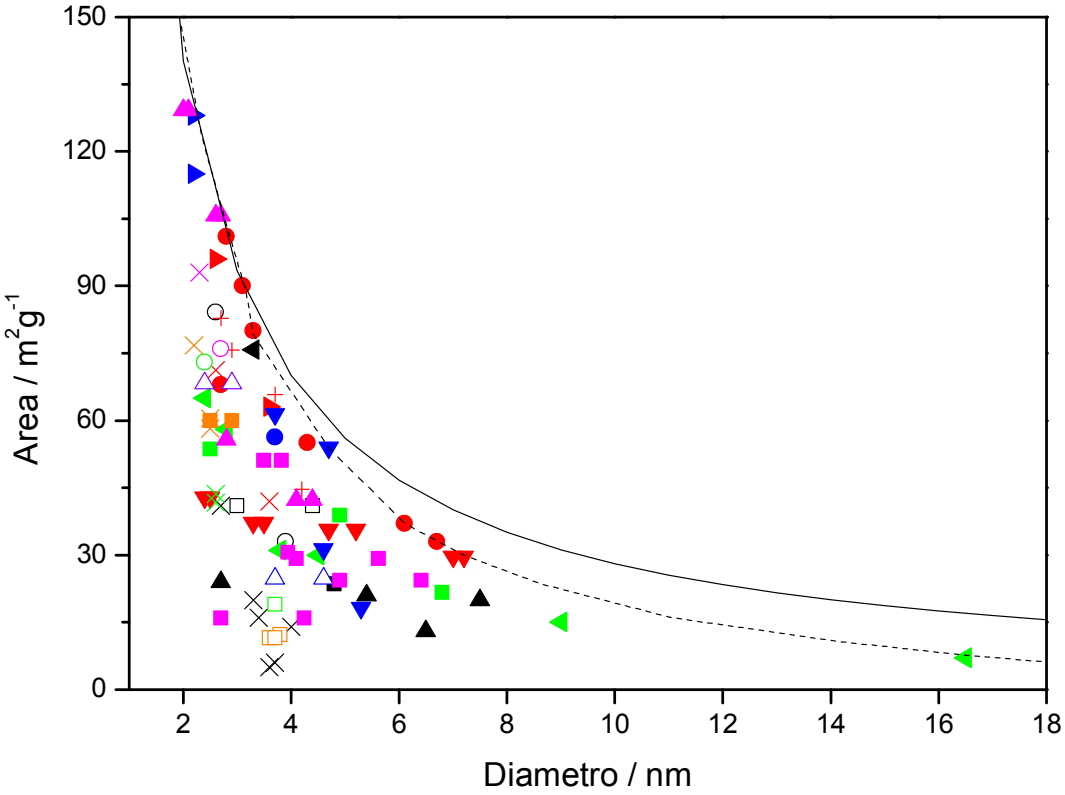
Formation of CO_2



Experimental motivation:

- Development and optimization of catalysts for fuel cells
- Graphene supported nanoparticles: measurement of the contact area





Preliminary results

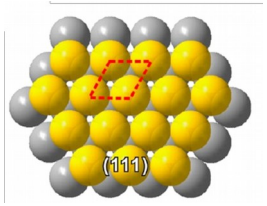
Contact area (A_c) of graphene supported nanoparticles

Contact distance ≥ Equilibrium distance (r_o)

$$\varphi(r) = \varepsilon[\exp(-2\alpha(r - r_0)) - 2\exp(-\alpha(r - r_0))]$$

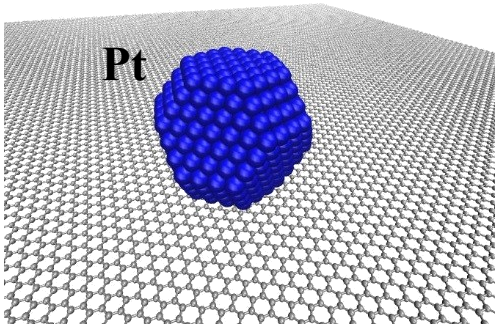
Area per atom (A_a):

$A_a = \alpha^2 \sqrt{3} / 4$

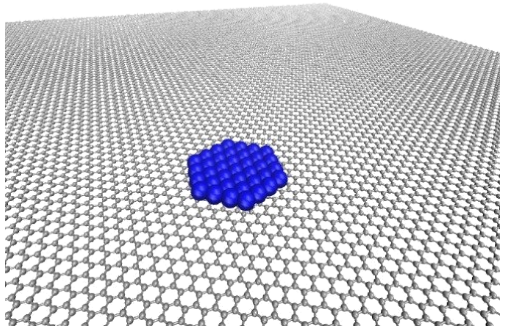


α = Lattice parameter

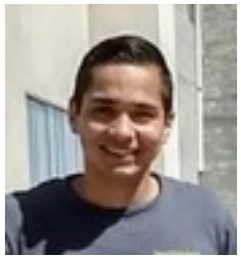
$A_c = A_a . N_{atoms}$



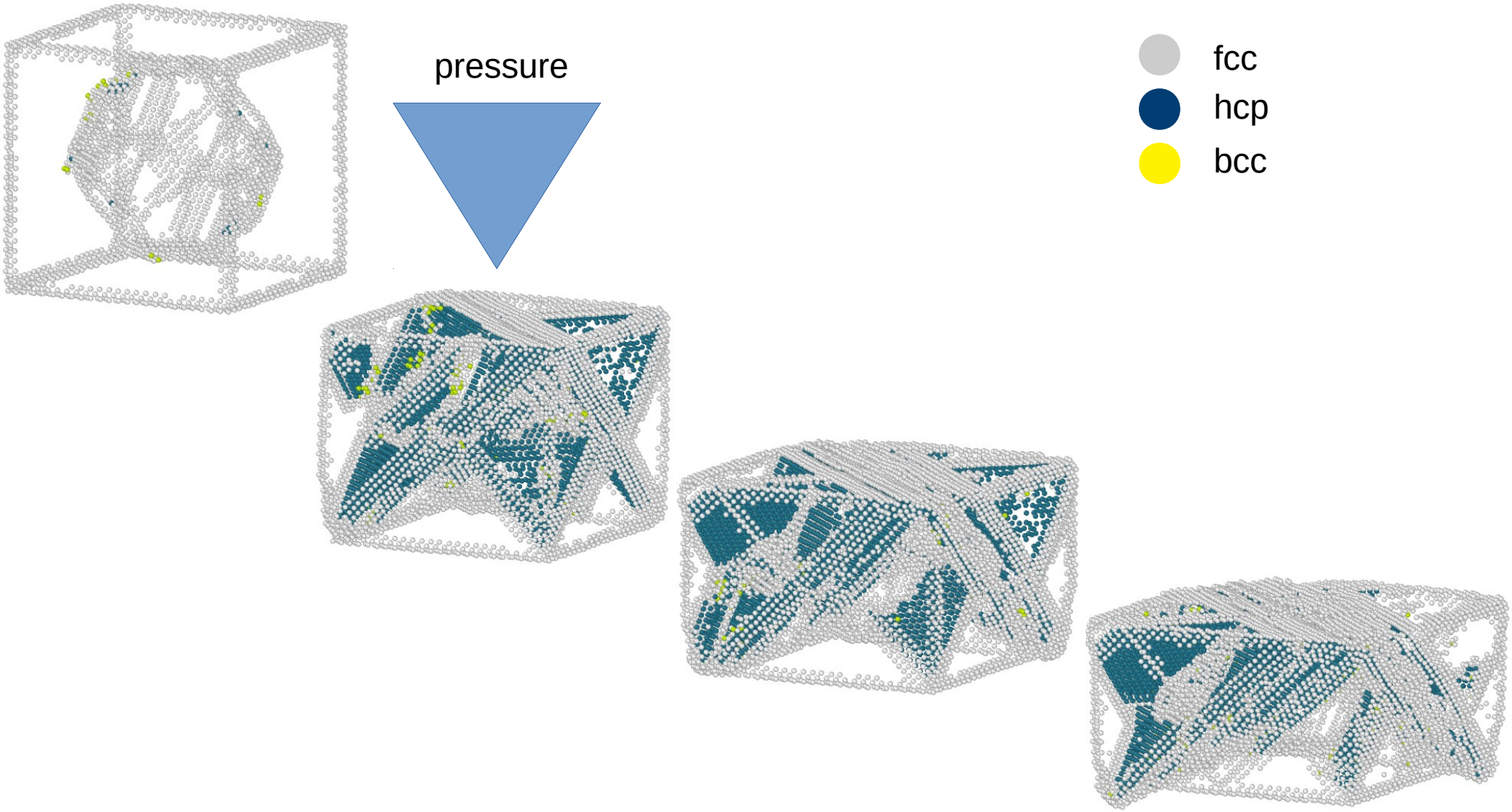
Cuboctahedron 586



A_c = 246.05 Å²



Mechanical properties of core-shell nanoparticles



2D materials as catalysts for fuel refining

Tomorrow!

TUESDAY (November 13)	
9:30 - 10:30	**Session E** Talk E1: Negreiros Talk E2: Maurice de Konig Talk E3: Helena Petrilli

New lightweight materials based on magnesium for the automotive technology

Global warming: We need to reduce CO_2 emanations

- Reducing the vehicles' weight
- Moving to alternative fuels

New lightweight materials based on magnesium for the automotive technology

Global warming: We need to reduce CO_2 emanations

- Reducing the vehicles' weight
- Moving to alternative fuels

Lightest structural metal Excellent castability Abundant, sustainable Non toxic, recyclable	**Magnesium**	Very reactive Fast oxidation, explodes Soft, low ductility Hydride too stable

New lightweight materials based on magnesium for the automotive technology

Global warming: We need to reduce CO_2 emanations

- Reducing the vehicles' weight
- Moving to alternative fuels

Lightest structural metal
Excellent castability
Abundant, sustainable
Non toxic, recyclable

Magnesium

Very reactive
Fast oxidation, explodes
Soft, low ductility
Hydride too stable

How do we solve it?

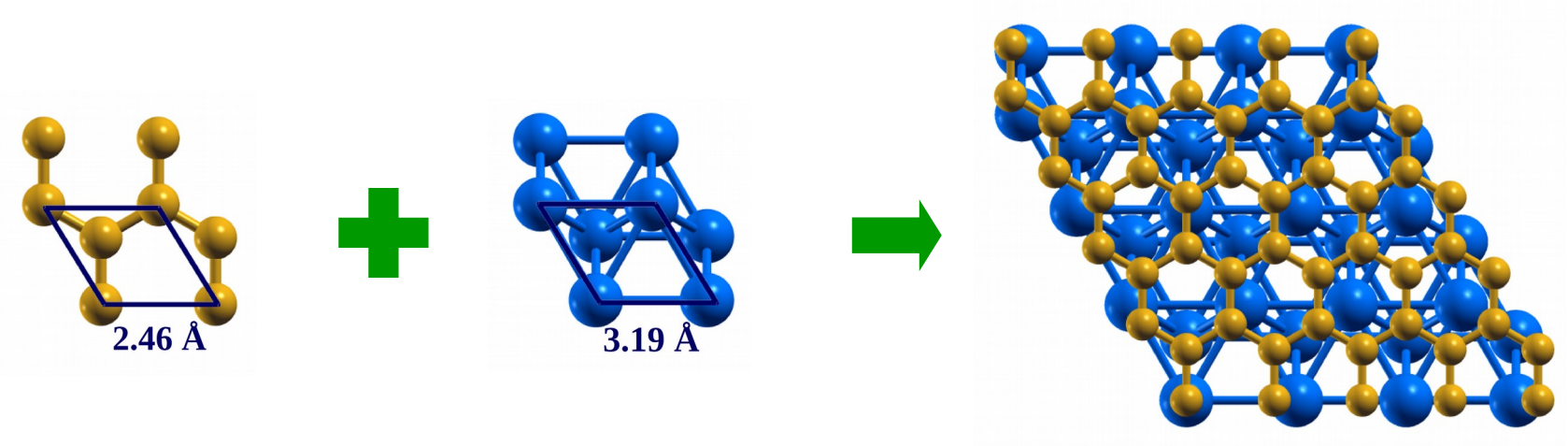
Main goals of our project

Massive alloys

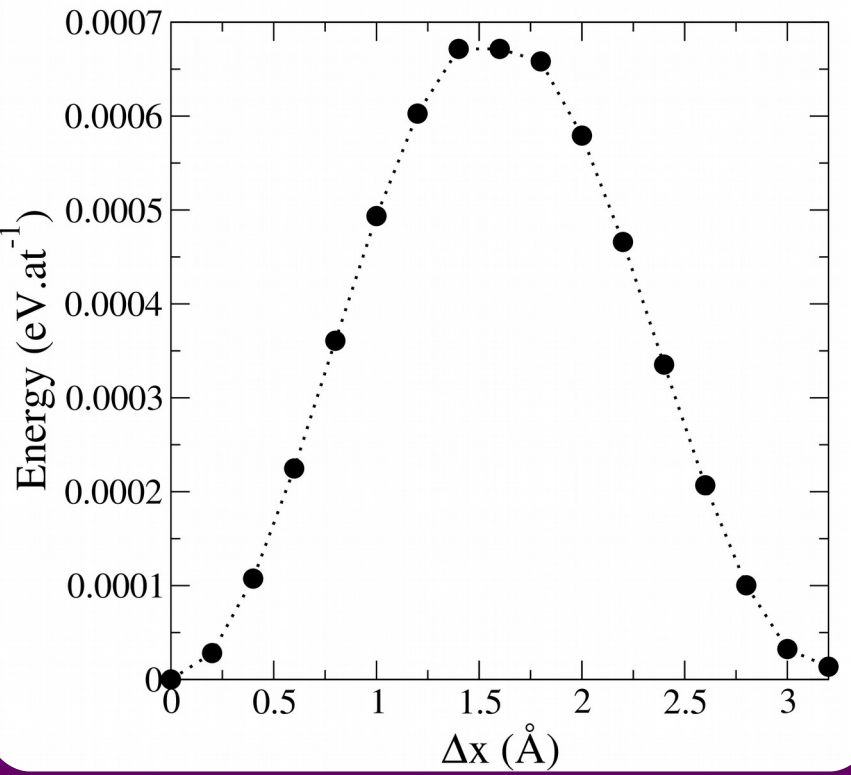
Heterostructures

Nanostructures

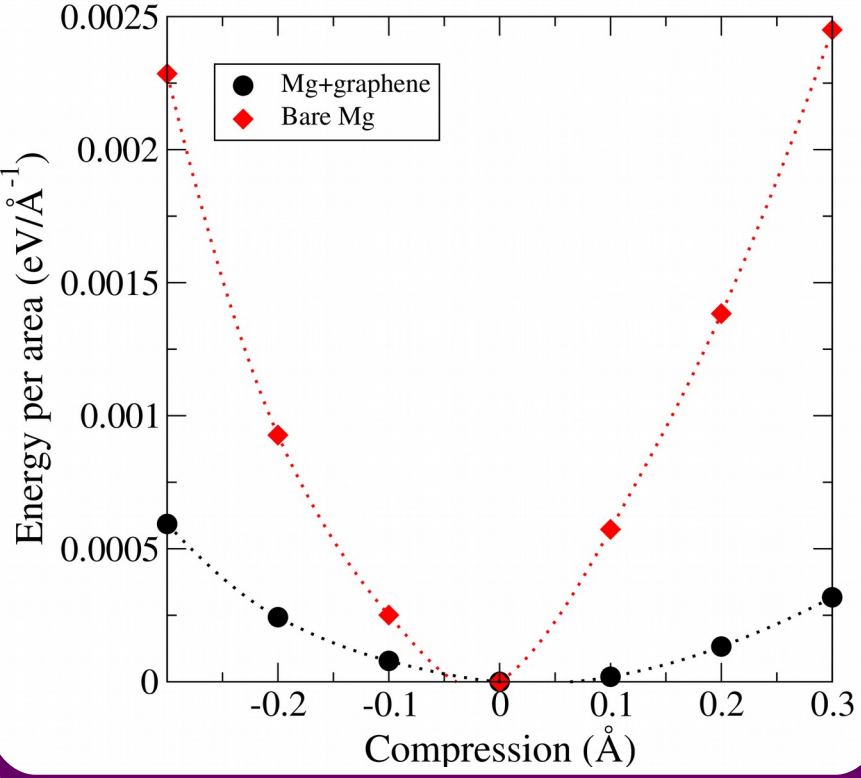
Mg-graphene heterostructures



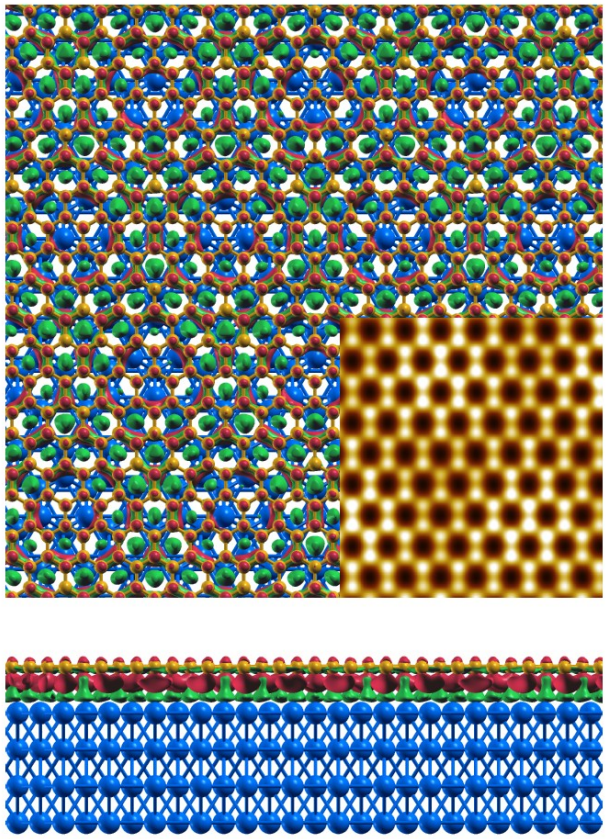
lubrication

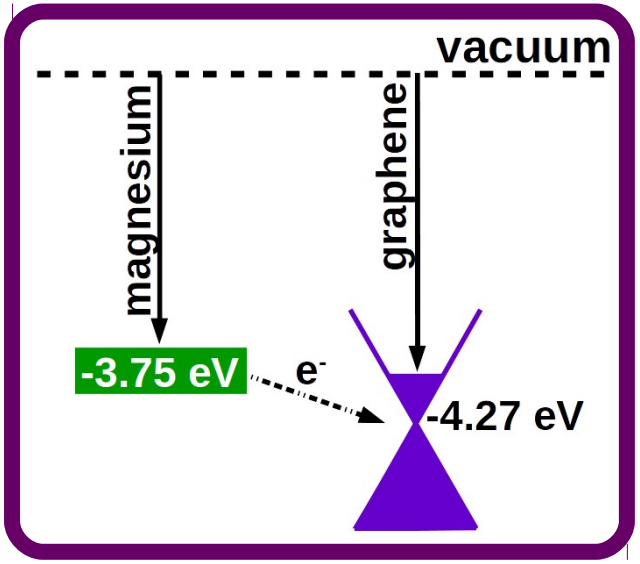


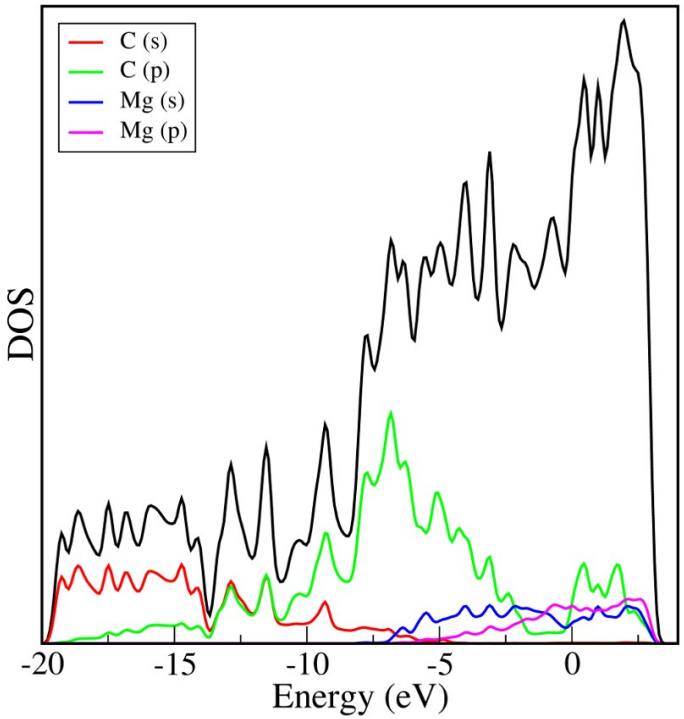
shock-absorption



Mg-graphene heterostructures





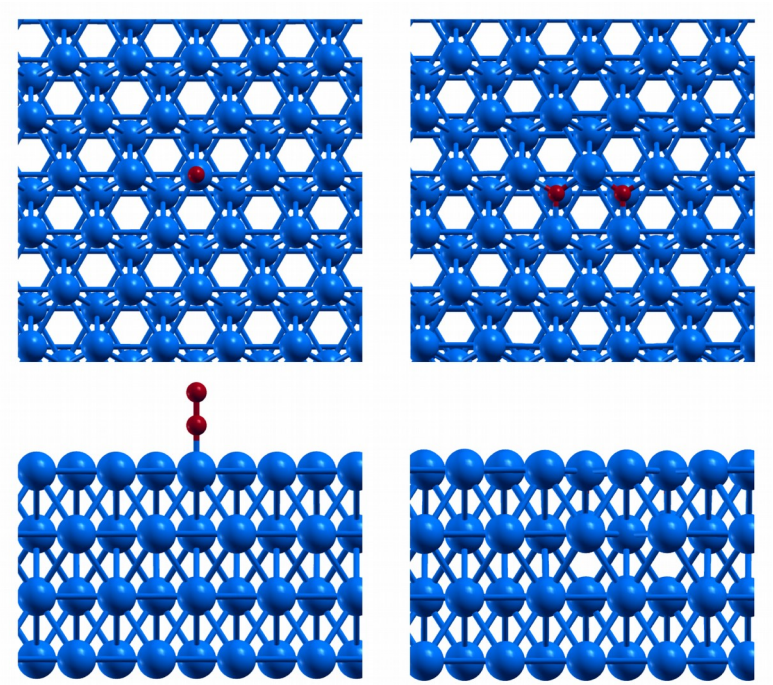


Charge transfer from magnesium to graphene

Magnesium oxidation

molecular

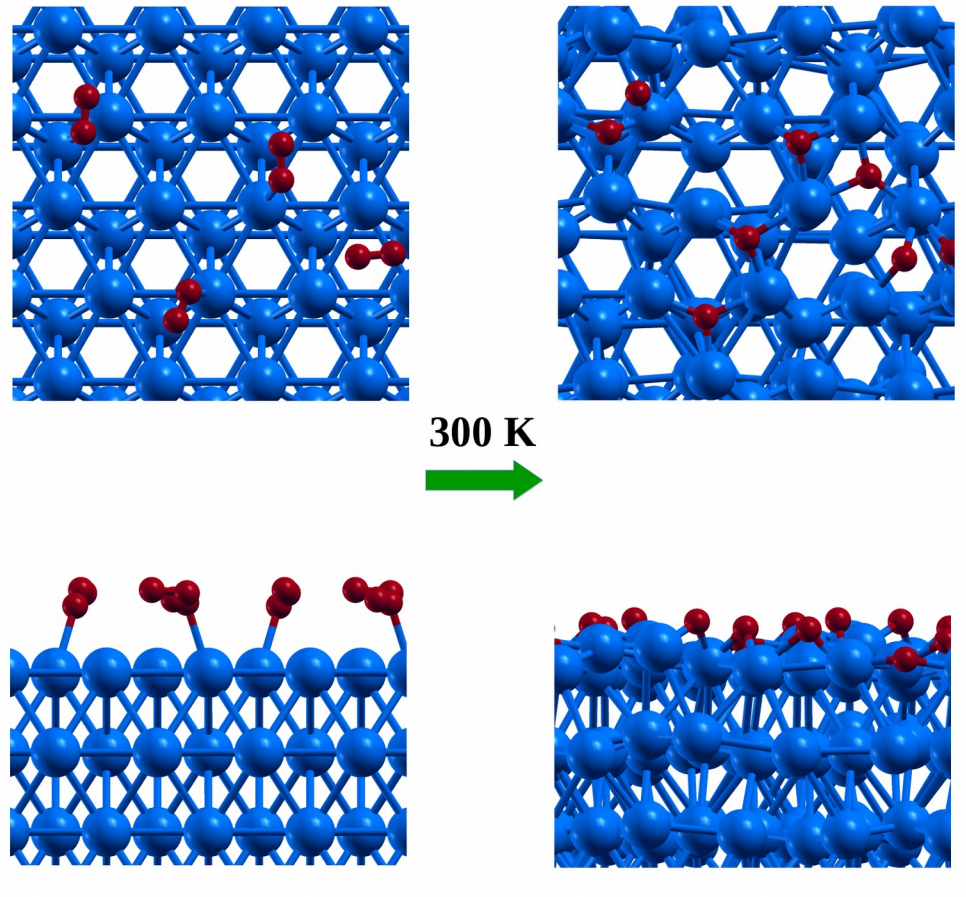
dissociatively



-0.57 eV

-4.47 eV

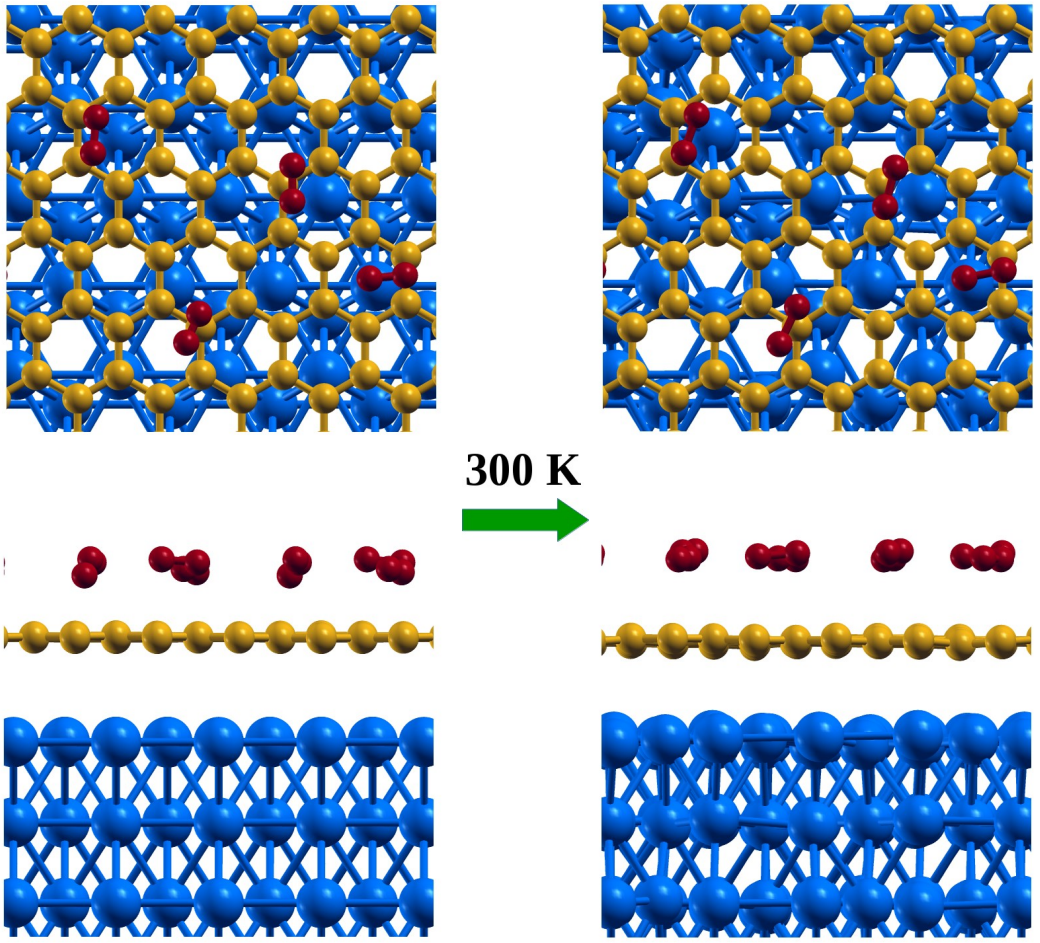
ab-initio MD simulation

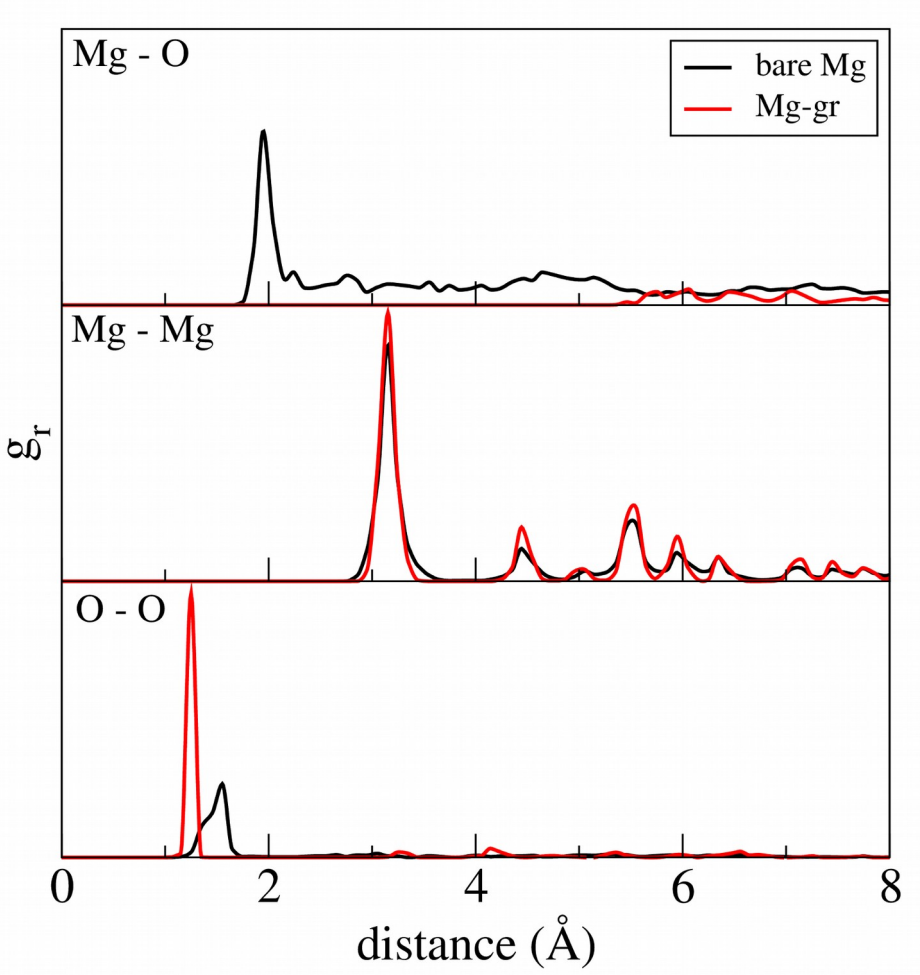


spontaneous fast oxidation

Avoiding oxidation

ab-initio MD simulation





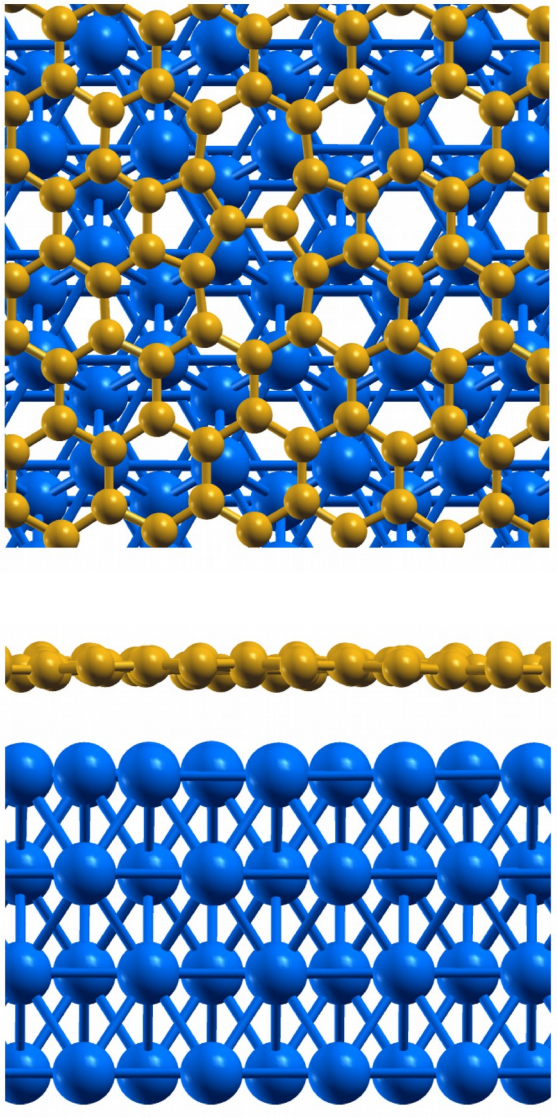
graphene covered magnesium does not oxidize

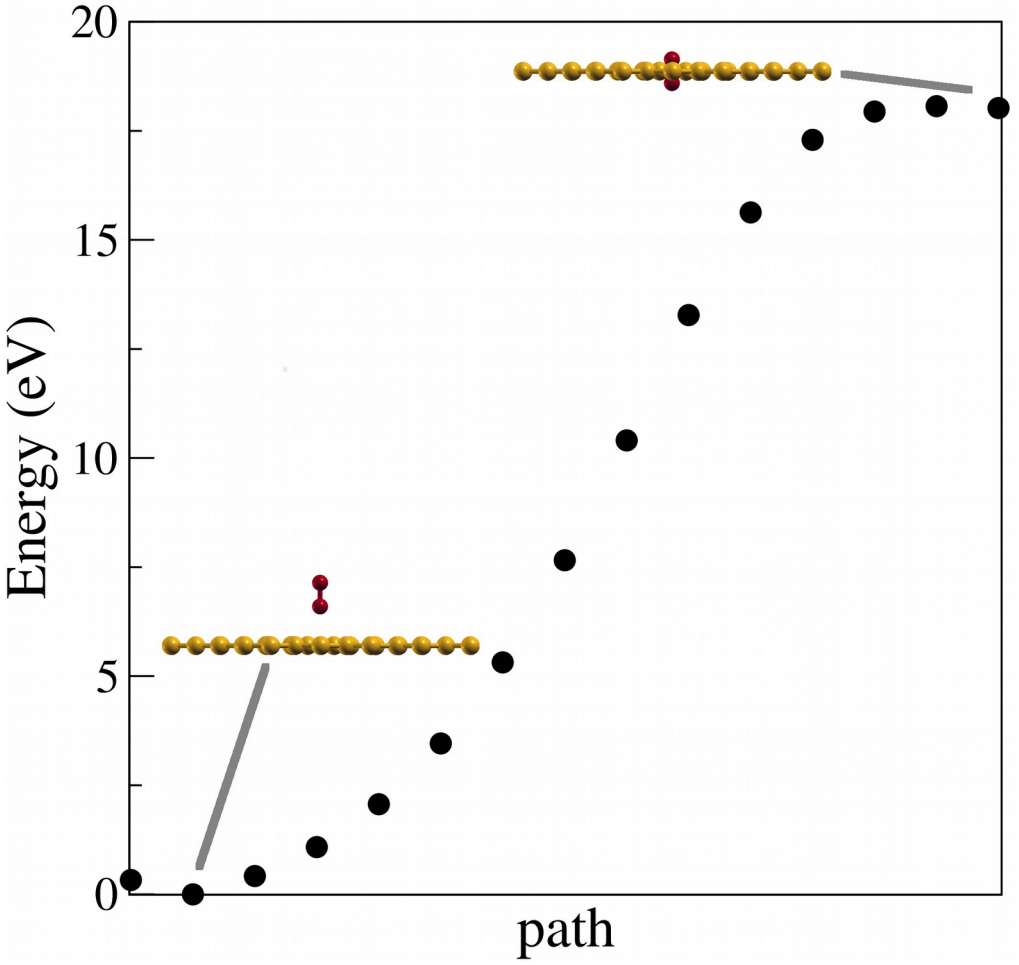
Real life: defective graphene

Experimentally, graphene may present defects

Real life: defective graphene

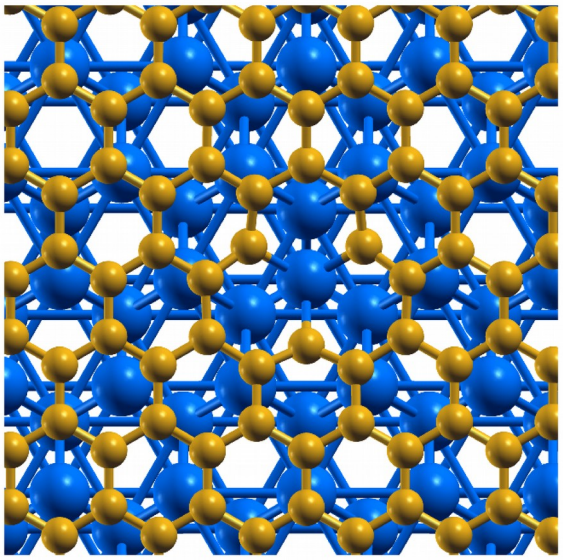
1) Stone-Wales defect

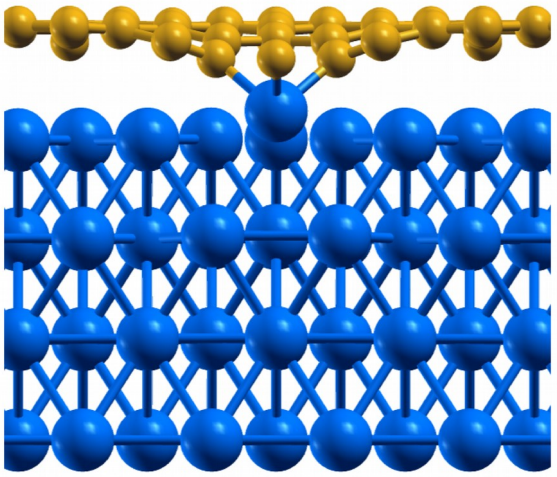




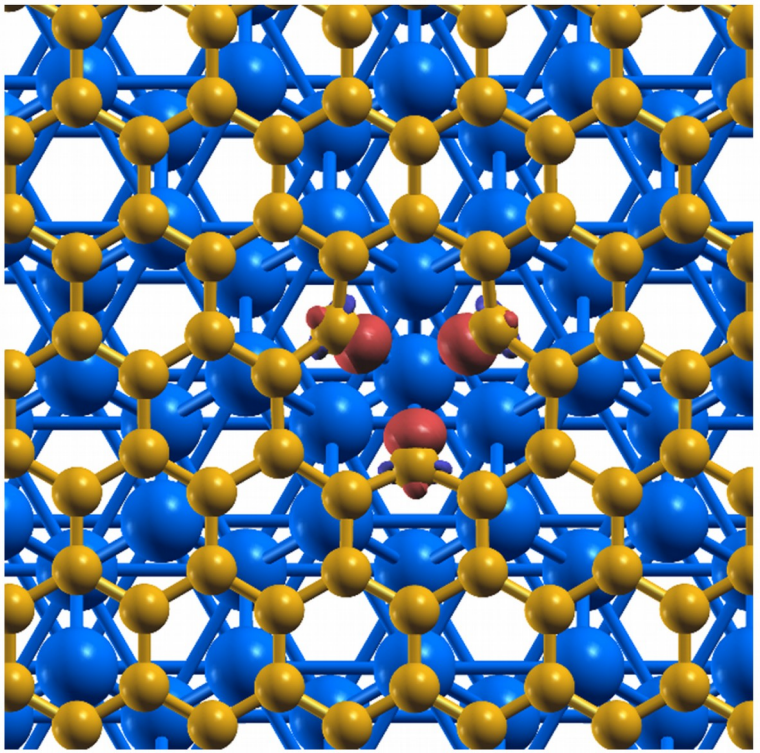
Real life: defective graphene

2) Single vacancy defect





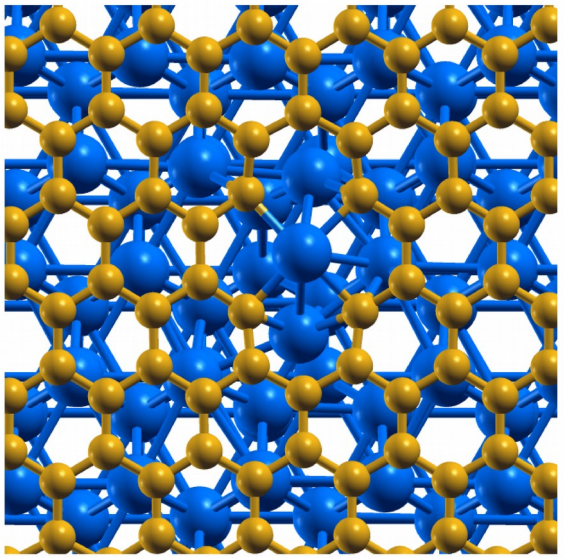
3 C-Mg covalent bonds are formed

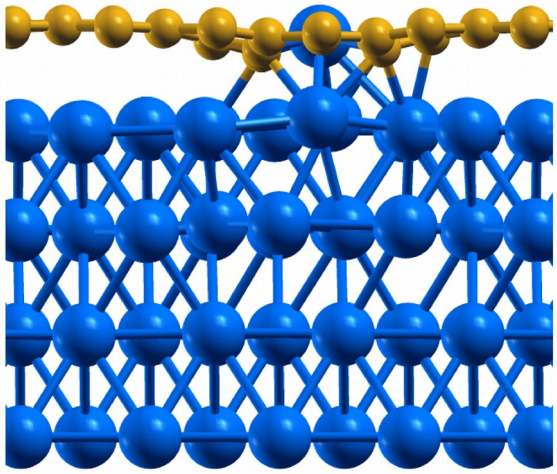


The exposed Mg atom does not oxidize

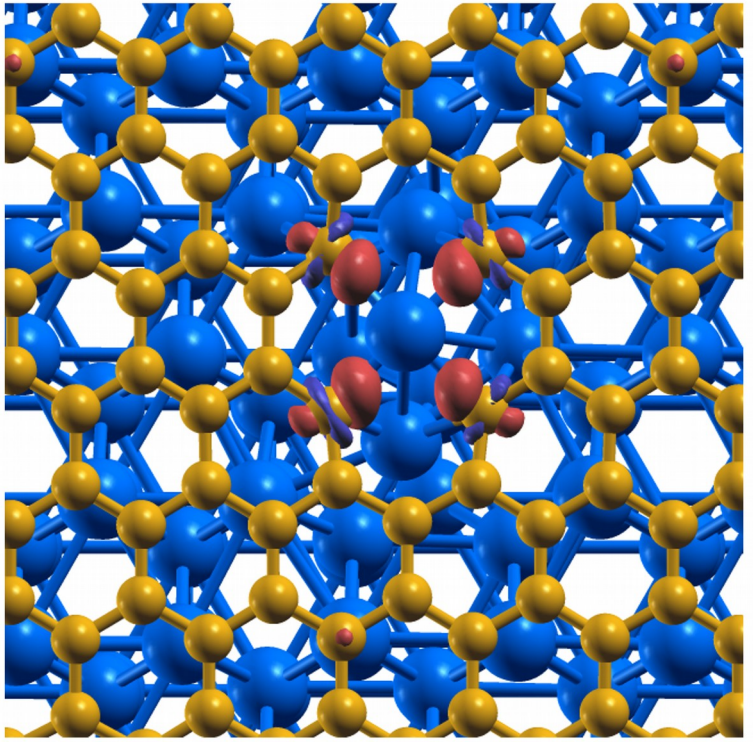
Real life: defective graphene

3) Double vacancy defect



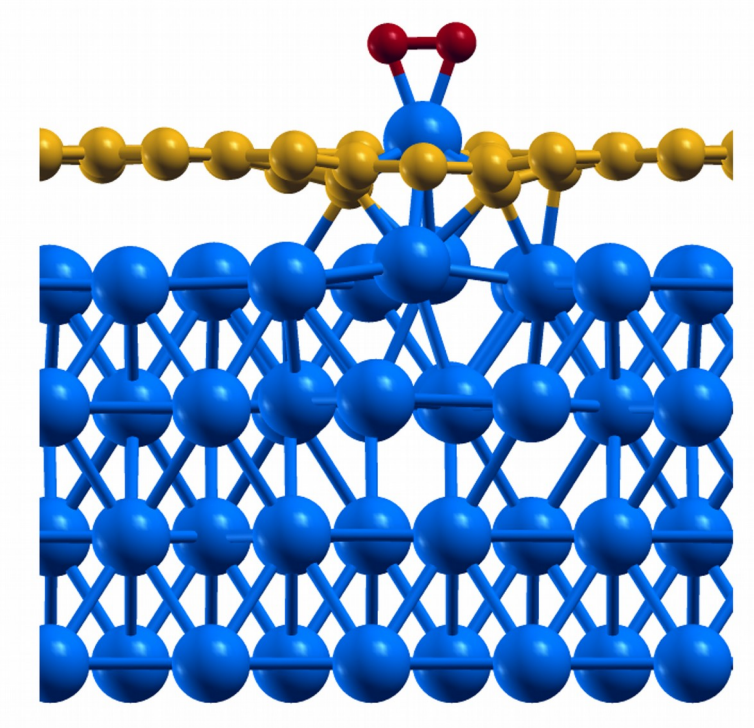


4 C-Mg covalent bonds are formed



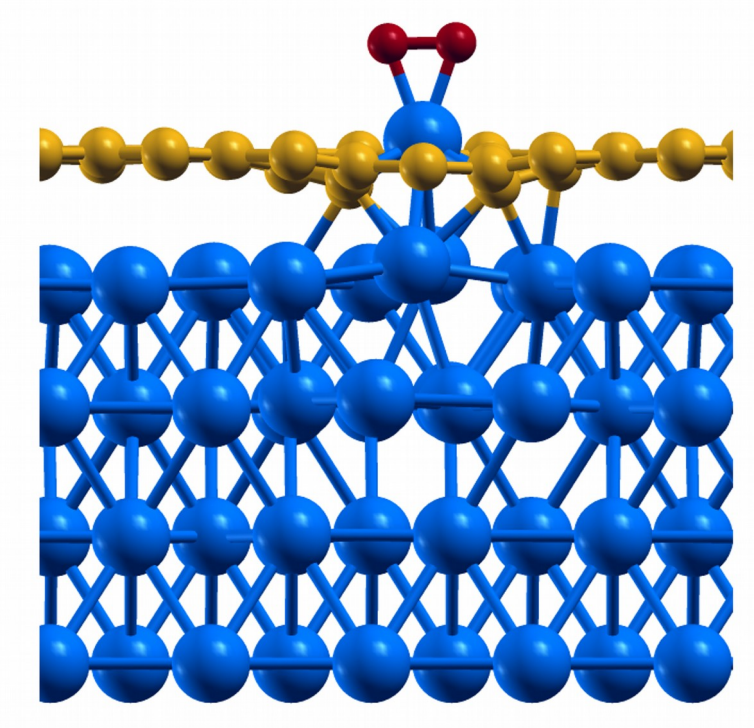
Real life: defective graphene

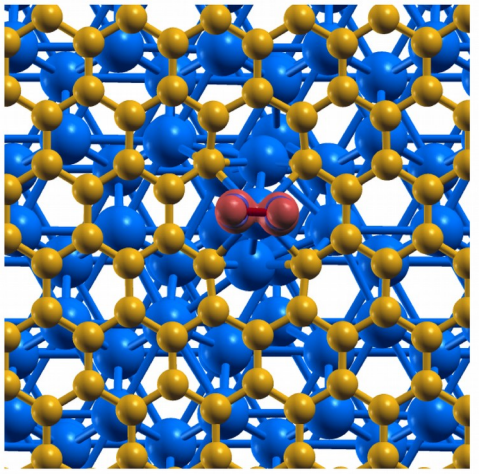
3) Double vacancy defect

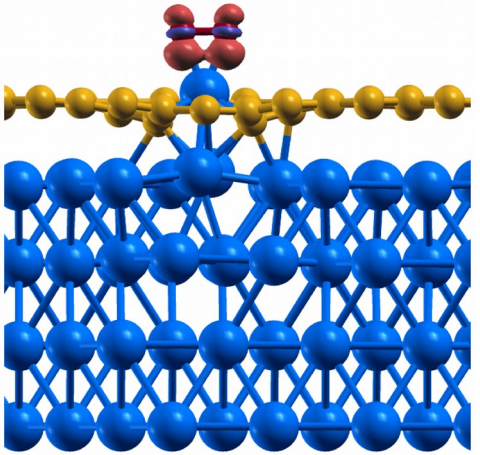


Real life: defective graphene

3) Double vacancy defect



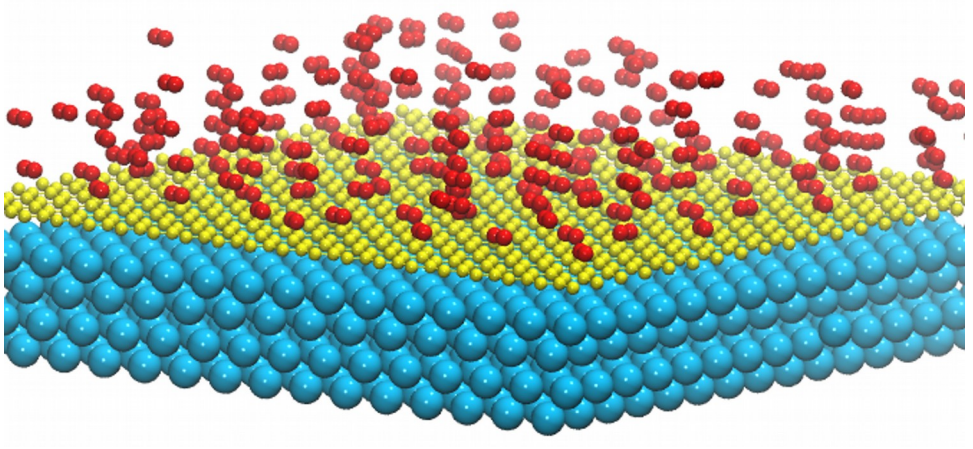




The exposed Mg atom oxidizes, but may protect the surface

Main conclusions

- **Magnesium-graphene heterostructures may be stable at room temperature**
- **The carbon monolayer, even defected graphene, acts as an efficient protection against oxidation**



Perspectives

Massive alloys

- Al-Mg Global minimum structure for different compositions
- Al-Mg-Zn Global minimum structure for different compositions
- Mechanical properties of selected structures
- Mg-C alloys

Heterostructures

- 2D heterostructures with other passivants
- Mg interaction with other carbonaceous materials

Nanostructures

- Nanoalloys of different compositions
- Mechanical properties of selected structures
- Support on different carbonaceous materials
- Hydride formation

Thank you!

Muito obrigada!

¡Muchas gracias!