Numerical simulation of matter at the nanoscale

Maria Peressi

Who:

presently with: Srdjan Stavrić (post-doc),
Simone Del Puppo, Davide Bidoggia (PhD students)
Walter Zuccolin (MSc student), Mario Spirito (BSc student)

Farnesina
Ministero degli Affari Esteri
e della Cooperazione Internazionale
Progetti di Grande Rilevanza

FERMAT
grant 2017KFY7XF

What:

- systems: graphene and low-dimensional systems, nanostructures, heterostructures (and moirè), surfaces, supramolecular assemblies
- properties: structural, electronic, magnetic, thermodynamical, chemical reactivity

With: mainly quantum mechanical approach;
ingredients: ions & electrons and interactions

QUANTUMESPRESSO

Where:

- "number crunching" on parallel machines: somewhere;
a few simulations and some post-processing: locally

CINECA

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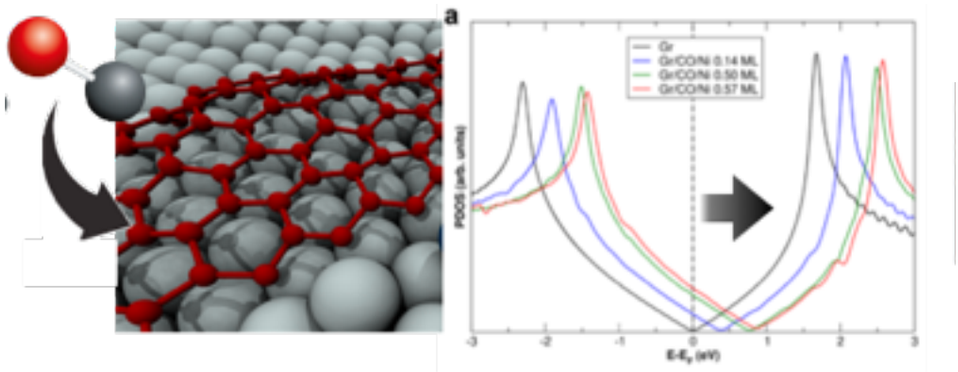

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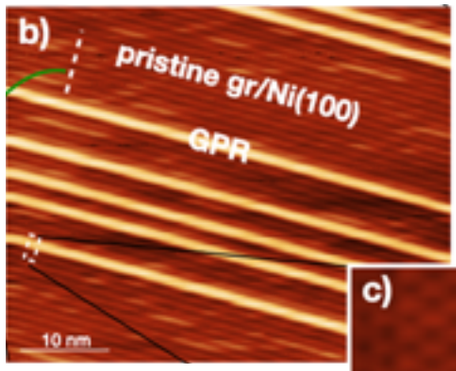
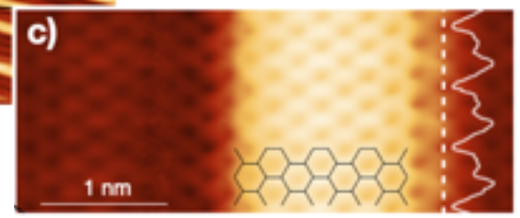
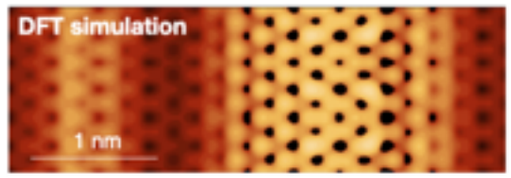
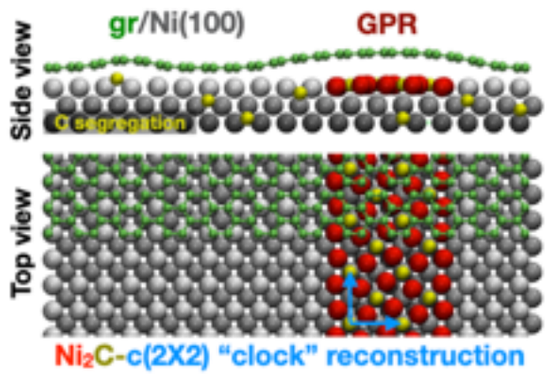
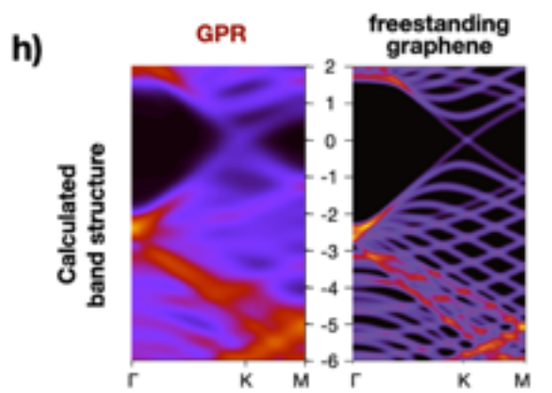


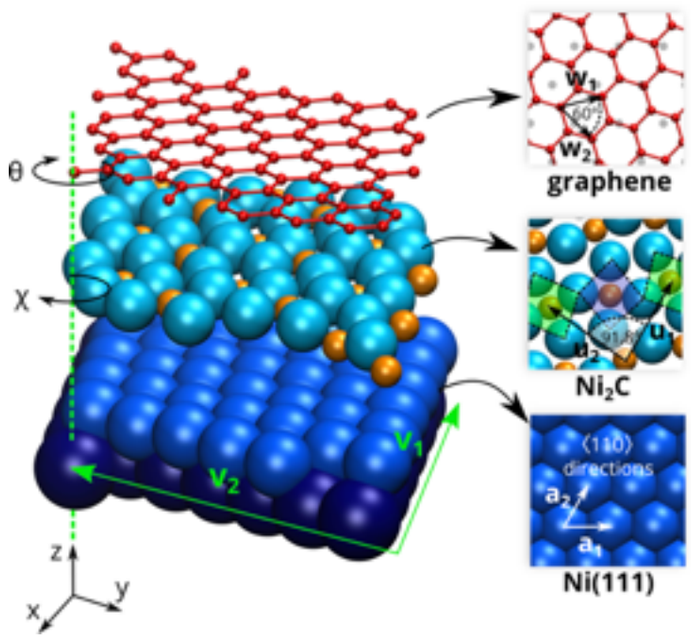


graphene and low-dimensional structures









graphene-based heterostructures and moiré

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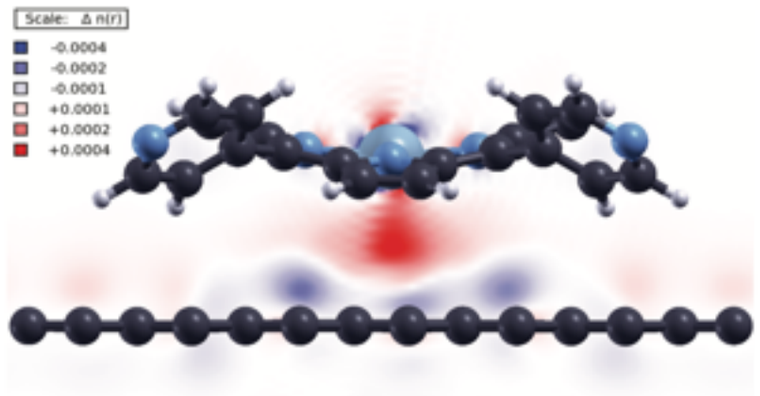
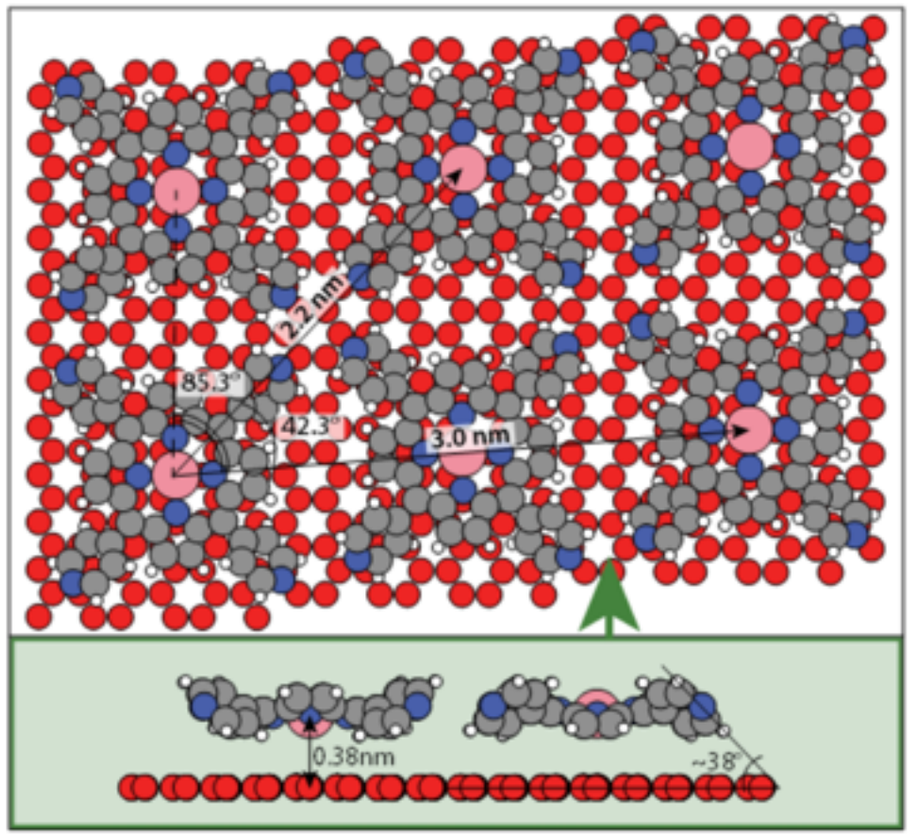


supramolecular assemblies



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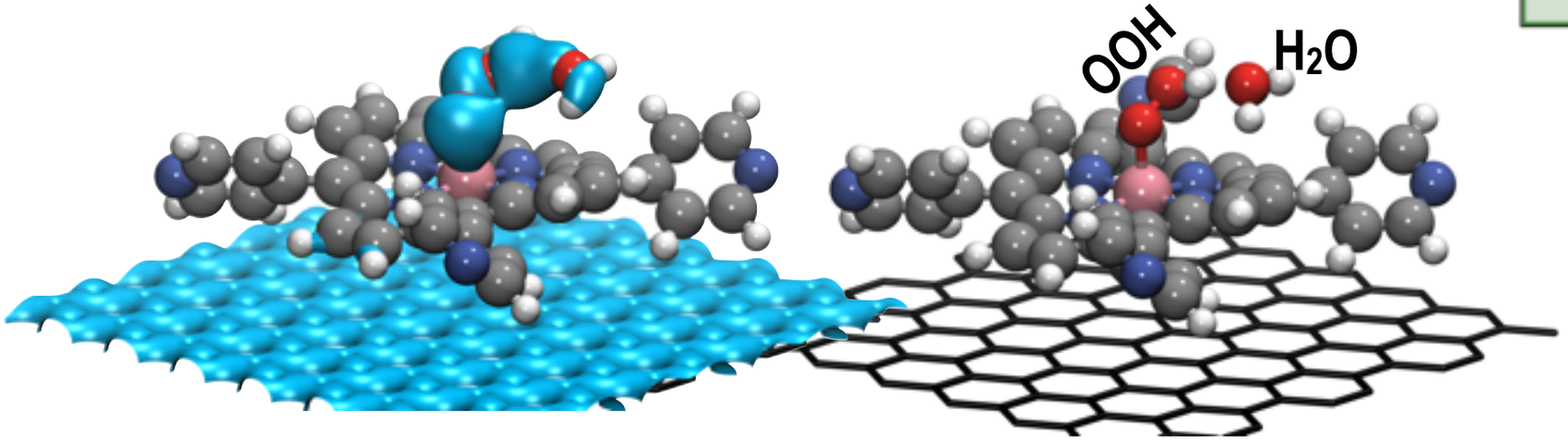

chemical reactivity