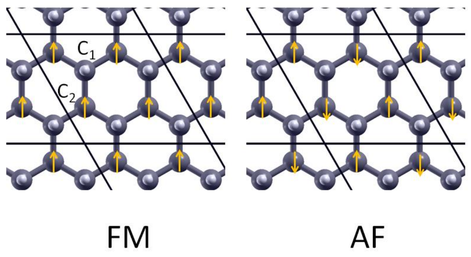
Computational Materials Science

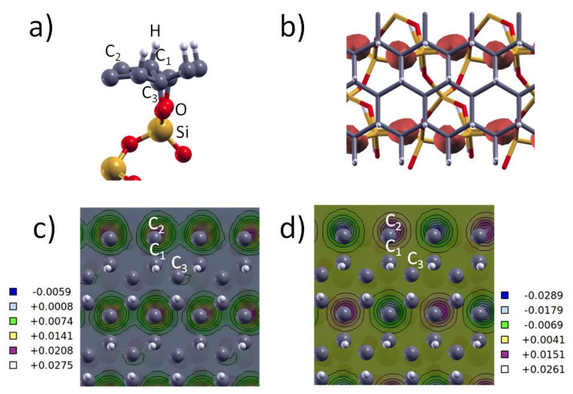
Materials for Nanotechnology

2D Magnetism



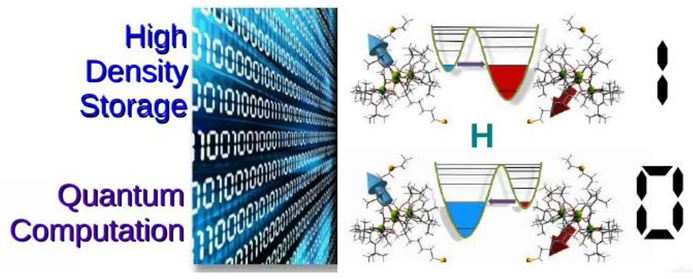
Graphone spin ferromagnetic and anti- ferromagnetic states. Arrows up and down stands for the electron spin polarization.

Graphone is a semi-hydrogenated derivative of graphene. Our ab initio calculations performed on CRESCO4 showed that spin polarization is reduced by ½ and ¼ when graphone is interfaced to copper or silicon oxide (substrates candidates for integration in real devices), respectively [Physica E, **78**, pp. 65-72 (2016)].

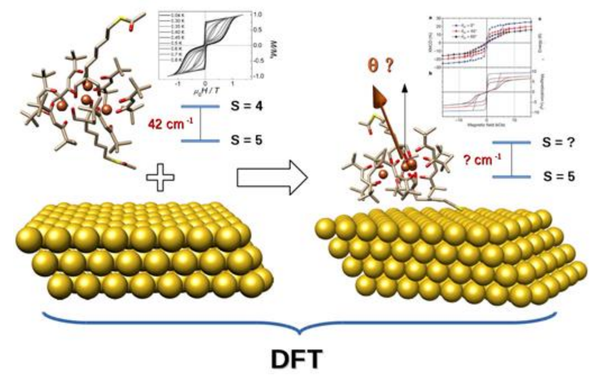


a) graphone adsorbed to SiO_2 surface; b) charge density difference (positive values are in red); spin density color maps of c) FM and d) AF states.

Magnetic Molecules

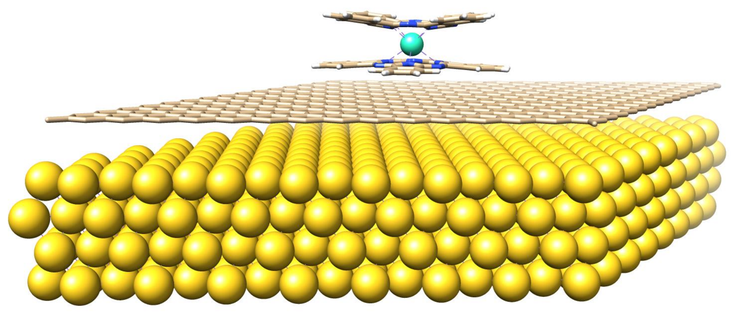


In order to be integrated into real devices, single molecule magnets (SMMs) and single ion magnets (SIMs) must show enough robustness upon grafting or absorption on surfaces. We showed the influence of the surface on several magnetic molecules once interacting with the different surfaces [Coord. Chem. Rev. **289-290** pp 357-378 (2018)].



Perspectives in Data Storage and Spintronics

SMMs, SIMs and graphone represent some of the best candidates to be used for magnetic data recording and in spintronic devices in general, though up to now only at cryogenic temperature. ENEA and LAMM will exploit CRESCO6 cluster to perform theoretical investigations of magnetic molecules and graphene derivatives interactions, paving the way to the development of heterogeneous organic-inorganic magnetic devices.



$TbPc_2(OC_{11}H_{21})_8$ adsorbed on graphene@Au(111)

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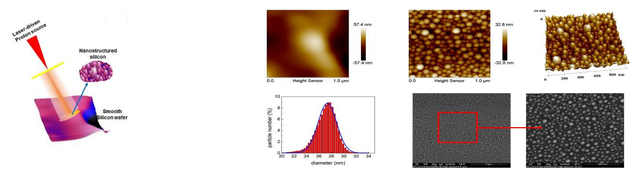
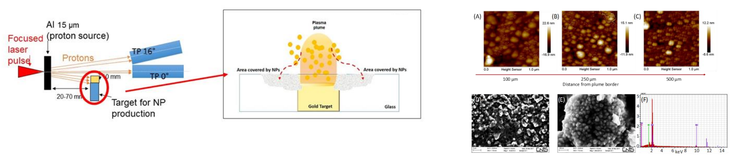
Nanocrystals and Nanostructure by Laser-Accelerated Protons

Laser-driven proton acceleration, as produced during the interaction of a high-intensity, short pulse laser with a solid target, is a prosperous field of endeavor for manifold applications in different domains, including astrophysics, biomedicine and materials science. These emerging applications benefit from the unique features of the laser-accelerated particles such as short duration, intense flux and energy versatility, which allow obtaining unprecedented temperature and pressure conditions.



Sketch of the experimental setup and AFM / SEM images



Computational Details

Classical Molecular dynamics

- 200.000 Silicon atoms;
- Simulated surface side ~ 280 Å;
- Simulation time > 1,5 ns;
- Modified Tersoff interatomic potential.

LAMMPS code on Cresco 4/5. Typical run uses hundreds/thousands of cores and several tens of GBs of disk space for I/O on parallel filesystems.

Classical Molecular dynamics

- 4.000.000 Gold atoms;
- Simulation cell side ~ 415 Å;
- Simulation time 600 ps;
- EAM - Embedded Atom Model interatomic potential

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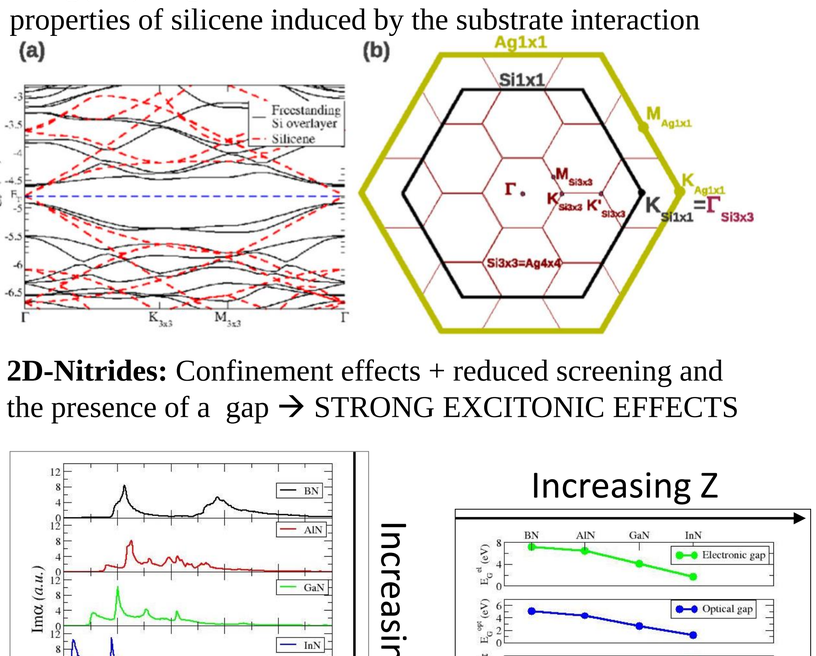
Results



Silicene: applications

Silicene, similarly to its 'cousin' graphene, is predicted to be endowed with many outstanding electronic and optical properties, such as massless Dirac fermions, absorbance going to a universal limit value of $\pi\alpha$ in the infrared region.

In addition, silicene-based devices might be most easily integrated than graphene with currently existing silicon electronics.

The issue of devising proper substrates to grow silicene is still open.

2D-Nitrides: applications

-Bulk group III-Nitrides AlN, GaN and InN are most important materials for solid-state lighting and solar cells. A central tool for band gap engineering is the alloying of GaN and or AlN with InN, extending the emission of nitrides based LEDs from UV to visible and IR region (*2014 Nobel prize in physics for the invention of blue LED awarded to Akasaki, Amano e Nakamura*).

-Why 2D Nitrides? Strong confinement effects open the way to new possible applications of these materials for light harvesting.

Models / Cresco resources

-Calculations performed within Density Functional Theory (DFT) and Many-Body Perturbaton Theory (MBPT).

-DFT Quantum Espresso code (www.quantum-espresso.org).

-GW CHISIG code, developed within the ETSF network (www.etsf.eu).

-Large supercells, especially to study silicene on Ag(111) substrates (up to 180 atoms/cell) → large parallelization and memory needs.

-Large number of k-points to obtain well-converged optical spectra (e.g. 200x200 k-points for freestanding silicene) → up to 1024 parallel processors, memory of 4 GB/core.

-Both requirements satisfied by **CRESCO4** resources.

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-O. Pulci, M. Marsili, V. Garbuio, P. Gori, I. Kupchak, and F. Bechstedt, Phys. Status Solidi B 252, No. 1, 72–77 (2015).

-M. Stella Prete, A. Mosca Conte, P. Gori, F. Bechstedt, and O. Pulci, APL 110, 012103 (2017)

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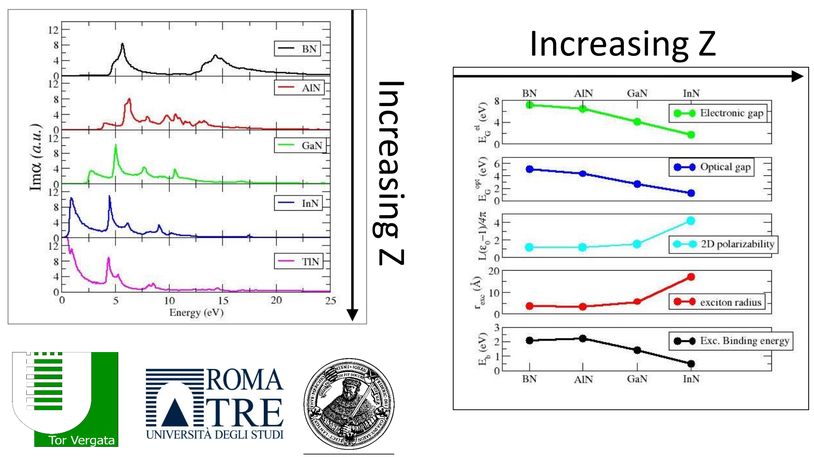
Results

Si/Ag(111): Significant modifications of the ideal electronic properties of silicene induced by the substrate interaction

2D-Nitrides: Confinement effects + reduced screening and the presence of a gap → STRONG EXCITONIC EFFECTS



Computational MAterials Science & Technology (CMAST) Virtual Lab http://www.afs.enea.it/project/cmast/