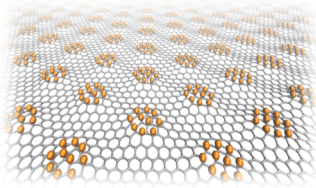
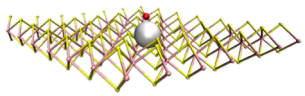
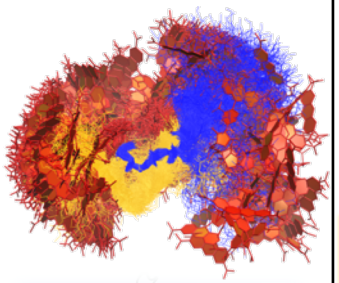
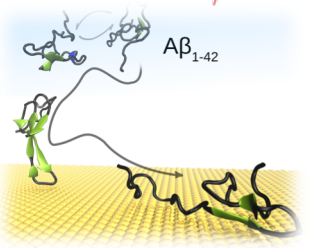
Molecular modeling and simulation: available Thesis projects

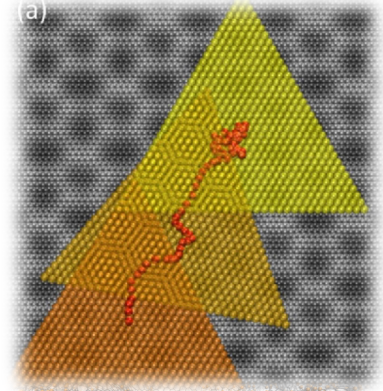


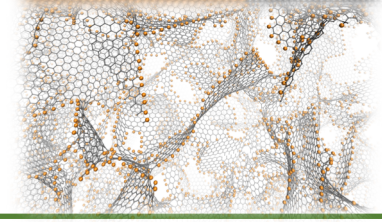


ab initio (DFT) simulations	Classical Molecular dynamics	Low resolution (coarse grained) models
Permeability of WS_2 membranes	**Suspended 2D materials**	
Unifiable in a single PhD project: Electronic properties of inhomogeneously deformed graphene	Structural properties of inhomogeneously deformed graphene	
Extendable to a PhD project: Reactivity of the Buffer Layer of graphene on SiC	Superlubricity of WS_2 on graphene	
Supported 2D materials	Formation proces of the QFSM	
	Electrolytes confined on electrodes	**Surfaces, porous strucutures, diffusion**
	Nanoporous graphene based scaffolds	Diffusion within nanoporous graphene
New fluorescent proteins in near infrared	Interactions between inorganic surfaces and biomolecules	Phase diagram of functionalized NPs
Biomolecular systems	Simulation of a FRET couple	Phase diagram of evolutionary switches

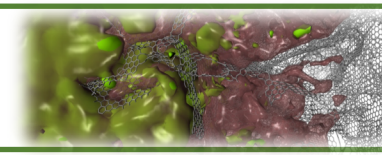




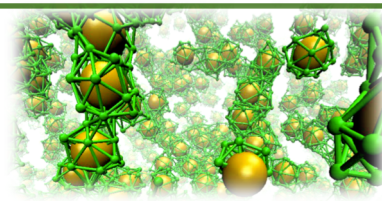


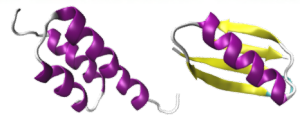


Extendable to a PhD project



Unifiable in a single PhD project





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Title	Tutors	Description and notes
Reactivity of the Buffer Layer of graphene on SiC	Valentina Tozzini Luca Bellucci	Study of the reactivity of the different superficial sites of the system towards different reactions (starting from H_2 adhesion). Links with experimental activity @NEST (S Heun). Use of HPC systems (local access and/or CINECA). Extendable to a PhD project for the functionalization of the layer to build multilayered structures
Permeability of WS_2 membranes	Valentina Tozzini	Study of the permeability of WS_2 membranes of increasing size with respect to different gases (e.g. He, possibly comparison with graphene membranes). Link with experimental activity (groups Univ Jena, Canberra, Bergen). Use, of HPC systems (local access and/or CINECA)
Properties of new fluorescent proteins in near infrared	Riccardo Nifosì	Molecular modeling of fluorescent proteins derived from photoreceptors to investigate the structure-fluorescence relationship, with classical and possibly hybrid (QM/MM (*quantum mech/molecular mech*) molecular dynamics techniques. Links with experimental activity @NEST and with theoretical groups @Univ Twente (NL)
Electronic properties of inhomogeneously deformed graphene	Valentina Tozzini	Study of electronic structure and reactivity of inhomogeneously and anysotropically streched graphene. Link with experimental activity @dip Fisica Pisa, within a PRIN project (PI prof Tredicucci). Use of HPC systems (local access and/or CINECA).
Structural properties of inhomogeneously deformed graphene	Valentina Tozzini Luca Bellucci	Study of the structure and dynamics of membranes of graphene subject to inhomogeneous and anisotropic distortion fields. Link with experimental activity @dip Fisica Pisa, within a PRIN project (PI prof Tredicucci). Use of local HPC systems, directly accessible. Unifiable with the previous for a PhD project
Superlubricity of WS_2 on graphene	Valentina Tozzini	Study of the dynamics activated either thermally and/or with external fields of triangular WS_2 on graphene. Study of the friction between WS_2 and graphene in different conditions. Links with experimental activity @NEST (Coletti, Forti). Use of local HPC systems, directly accessible.
Formation of the quasi-free standing graphene	V Tozzini L Bellucci R Farchioni	Study of the hydrogen intercalation underneath the buffer layer. Optimization of the force fields for the interaction with hydrogen and/or use of reactive force fields Links with experimental activity @NEST (Heun/Veronesi). Possible extension to include lithium intercalation for a PhD project
Electrolytes confined on electrodes	Luca Bellucci Valentina Tozzini	Study of the structure and dynamics of the electrolyte layers near the surface of a charged electrode. Effect of confinement on the diffusion, vibrational dynamics and thermal conducibility. Link with experimental activity @NEST (Heun/Veronesi). Use of local HPC systems, directly accessible.
Interaction between inorganic surfaces and biomolecules	Luca Bellucci Valentina Tozzini	Study of the interaction between biomolecules (proteins or peptides) and inorganic surfaces or nanoparticles, possibly functionalized. Exploration of the conformational space and adsorption with advanced sampling techniques (Replica Exchange or metadynamics). Use of HPC systems (local access and/or CINECA).
Simulation of a FRET pair (*Fluorescence resonant energy transfer*)	Riccardo Nifosì	Study of the distance between two proteins connected by a peptide linker, for the calibration of the experimental measure of proteins distance by FRET. Molecular dynamics atomistic simulations with enhanced sampling (*Replica Exchange* or Metadynamics). Links with experimenta activity@NEST (Storti, Bizzarri).
Nanoporous graphene based scaffolds	Luca Bellucci Valentina Tozzini	Modeling of 3D nanoporous scaffolds based on graphene, or (reduced) graphene oxide and/or functionalized for the adsorption of gas/fluids (for supercaps, hydrogen storage, batteries), filtering or catalysis. Development of computational protocols and codes for building and characterization of the models. Integrable with the following for a PhD project.
Diffusion in nanoporous graphene	Luca Bellucci Valentina Tozzini	Study of diffusion of electrolytes and/or other fluids/gases in disordered 3D graphene scaffolds with different porosity. Phase diagram for the diffusion as a function of the size/charge of the particles, possibly represented at the coarse grained level. Machine learning algorithms for the exploration of the parameters space. Use of local HPC resources and/or CINECA.
Phase diagram of functionalized nanoparticles (NP)	Valentina Tozzini	Study of aggregation of gold nanoparticles functionalized with hydrophobic residues as a function of their size, charge, concentration and temperature, with low resolution models. Collaborations with NANO-Modena and Technological Univ Dublin. Use of local HPC systems.
Phase diagram of evolutionary switches	Valentina Tozzini	Study of the helix-sheet transition in model proteins based on the evolutionary switches. Exploration of the phase diagram in the parametric and sequence space, with machine learning and genetic algorithms coupled to molecular dynamics. Collaborations with Moscow Univ, Saint Petersburg Univ, and CNRS Montpelleier. Use of local HPC resources.