DYNAMICS NANOMATERIALS WITH FUNCTIONAL PROPERTIES

Supervisor: Paola Posocco (University of Trieste)

The research activity will focus on studying self-assembling dynamic nanomaterials in equilibrium and out-of-equilibrium conditions to understand key molecular factors, forces and properties that control self-assembly, structure, reaction, adaptability, and recognition properties. Two main classes will be investigated by computational techniques and machine-learning approaches: peptide-based systems and organo-modified metal nanoparticles. Via the integration of classical atomistic and coarse-grained molecular simulations, advanced molecular simulation methodologies and data-driven models, the candidate will explore structure, dynamic and functional behavior of these fascinating nanomaterials on a wide spatio-temporal scale. The activity will be carried out in collaboration with national and international experimental groups.

The ideal candidate has a Master Degree in Chemistry, Physics or Materials Science. Basic experience with common molecular simulation packages (e.g. LAMMPS, GROMACS, AMBER) is required, along with reasonable programming skill (Python or Fortran). Strong motivation and enthusiasm for research, good attitude to work in team, good written and spoken English is also an asset.

REFERENCES

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- Luo, Z. et al.; Quantitative 3D Determination of Self-Assembled Structures on Nanoparticles Using Small Angle Neutron Scattering. *Nat. Commun.* **2018**, 9, 1343.
- Şologan, M. et al.; Patchy and Janus Nanoparticles by Self-Organization of Mixtures of Fluorinated and Hydrogenated Alkanethiolates on the Surface of a Gold Core. *ACS Nano* **2016**, 10, 9316.
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