Title	**Multiscale Modeling of Hybrid systems: Structure, Dynamics and Properties**
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Project description

Introduction

The need to improve materials performance at the nanoscale for applications in the engineering, biomedical, therapeutic, food, agricultural, environmental, etc. sectors has induced the scientific community to combine experiments with computational chemistry techniques, which are very effective for driving the research, reducing production times and costs. The computational resources available today have reached high levels of accuracy and have pushed the size and time scale limits to the nano/subnano and micro/nanosecond domains.

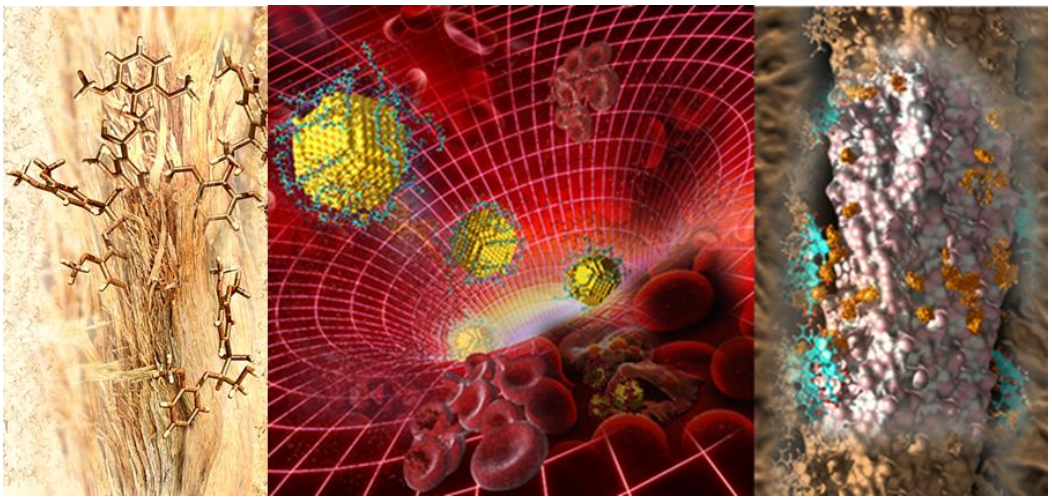

Figure 1. *Examples of computational models developed in our group. Wood components in solutions and on selected catalysts (recycling biomasses) [1], functionalized gold nanoparticles in the bloodstream (thermal therapy against cancer cells) [2], nanocellulose based eco-filters (i.e. to capture metal ions and dye contaminants) [3].*

Topics

The project will be focused on the design of multi-scale/level computational protocols, comprising quantum chemistry methods and simulation procedures based on force fields parametrized on purpose, for disclosing hybrid materials structure, dynamical behavior and response properties in various types of environments. Some suggested topics could be the following:

- the process of formation and growth of surfaces and nano-particles assemblies eventually covered with adsorbed molecular/macro-molecular species capable of protecting the growing system, tuning its morphology and response properties.
- polymeric and bio-polymeric matrixes properly functionalized to enhance mechanical and physico-chemical properties.

Skills and Expected Results

- Acquisition of the skills to model representative systems and realistic perturbations, selection of the most appropriate computational procedures to investigate the chosen system properties, implementations of new codes to improve the existing tools for simulating/calculating and analyzing the statistical data. Development of a critical view of the capabilities and limitations of each tool at their disposal.
- Characterization of the structure, dynamics, reactive properties of complex materials in realistic environments by disclosing the main interactions which role the behavior of the selected systems.
- At the end of the training period, the student will be capable of developing new ideas and translating them in research projects.

Publications

[1] **S. Monti**, P. Srifa, I. Kumaniaev, J. S. M. Samec *J. Phys. Chem. Lett.* **2018**, 9, 5233.
[2] **S. Monti**, V. Carravetta, H. Ågren *Nanoscale* **2016**, 8, 12929; **S. Monti**, V. Carravetta, H. Ågren *Small* **2016**, 12, 6134 (cover); **S. Monti**, **G. Barcaro**, L. Sementa, V. Carravetta, H. Ågren *Nano Research* **2018**, 11, 1757 (cover).
[3] C.Zhu, **S.Monti**, A.P. Mathew *ACS Nano* **2018**, 12, 7028.
[4] **G. Barcaro**, **S. Monti**, L. Sementa, V. Carravetta *J. Chem. Theory Comput*. **2019**, 15, 2010.
[5] **G. Barcaro**, L. Sementa, V. Carravetta, T. Yano, M. Hara, **S. Monti***, Phys. Chem. Chem. Phys***. 2019***,* 21*,* 5435.

Collaborations/Network

Prof. Adri C. T. van Duin – Department of Mechanical & Nuclear Engineering Pennsylvania State University, University Park PA 16802, **USA.**
Prof. Aji Mathew - Department of Materials and Environmental Chemistry, Stockholm University, **Sweden.**
Prof. Riccardo Ferrando and Prof. Giulia Rossi, Department of Physics, Genoa University**, Italy.**

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