CECAM-FR-MOSER Sponsored Event

Workshop on multiscale modelling of materials for 5th generation roads

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A. Introduction and motivation

The scientific research and related technology applications face nowadays-challenging problems concerning energy consumption, environmental impact and sustainability of the developed methodologies at the industrial and global scale. Material science, in particular, is concerned with the study of alternative materials able to enhance the present energy storage and energy supply technologies, reduce the environmental impact of the transportation based on fossil fuel, or improve the efficiency of the industrial devices, processes and equipment. In this context, the study of photocatalytic, photoluminescent and photovoltaic materials is promising and it is arousing interest in the scientific community. These new materials, so-called *smart*, could be added to traditional construction ones, in the form of additives dispersed into cements, concrete, asphalt, etc. to confer new and unconventional properties.

In the near future, photovoltaic technology applied to building materials will play a key role in the search of environment-friendly and renewable energy sources, while photocatalytic materials will be used to convert polluting molecules or greenhouse gases into harmless species. Provided that a convenient formulation for their integration into coatings or fillers is found (e.g. finely dispersed micronized particles, nanoparticles, active species supported on molecular frames, etc.), and the relevant molecular interactions with the surrounding environments are established, their use in building materials and roads may become routine in the forthcoming years. Another crucial aspect of material science is the storage and capture of greenhouse gases and the reduction of air pollutants, particularly close to urban areas. Catalytic control of air pollution has become an essential feature of the chemical process design and, among other positive outcomes, has led to a dramatic reduction of pollutant emissions in the exhaust gases of modern engines. The principal pollutants resulting from combustion of fossil fuels are, apart from non-oxidized or partially oxidized hydrocarbons, carbon monoxide (CO), nitric oxides (primarily NO, NO_2 and N_2O) and sulfur oxides. Nitric oxides are formed in combustion reactions when atmospheric nitrogen combines with oxygen at high temperatures. These simple gases have dreadful consequences for the environment and human health, so their emissions into the atmosphere should be constantly monitored and their concentrations reduced. A major threat to human health comes also from indoor air pollution. The air quality of indoor environments is difficult to monitor and control because of the multiple sources of pollution (building materials, consumer products, cigarette smoke etc.) and ventilation conditions. Among the main sources of indoor and outdoor pollution are halogenated hydrocarbons, like vinyl chloride and tetrachloroethylene, and simple amines. Nanocatalysis represents a novel and rapidly expanding field of research for the industrial chemistry and many examples of applications of nanostructured materials in both homogeneous and heterogeneous catalysis exist, where nanoparticles of oxides, metals and semiconductors are employed to synthesize important chemical products or intermediates or for degradation of contaminants and pollutants. The improvements of the reaction yields and selectivities, as well as the durability of the catalysts, are among the objectives and challenges of nanocatalysis. In particular, the possibility of using highly active nanocatalysts to conduct reactions, that would normally require high values of temperature and pressure, under mild conditions is particularly valuable.

Molecular modeling of such systems is challenging, since it must conjugate the accurate description of electronic structure properties at the molecular and nanoscopic level with the optical, electric and mechanical properties deduced at the mesoscopic and macroscopic

scales, thus requiring a close interplay between theories and models that have been devised for different length scales and systems. A multi-scale model should be found and implemented in order to connect all these scales.

B. Objectives

The aim of this 2 and half days workshop is to gather European and worldwide experts (academic and industrials) in electronic structure computations, molecular modeling, material science and those working on developing and implementing the new roads (Roads of 5th generation, RG5). Indeed, concerning the targeted systems, different points will be addressed, such as their importance (applications and implications), their production at the laboratory and industrial scale, the methods and approaches for the description of the properties of interest, and the economic, environmental and toxicological aspects. Thus, we will discuss together the needs of each community and define a common strategy to develop novel catalysts, sensors and photovoltaic devices for the future road construction and building.

Concerning the simulation tools, different sections will be devoted to:

- A half-day session will allow discussion of the computational aspects and results from standard existing procedures for the accurate description of electronic and mechanical properties of inorganic/organic active molecular systems and their substrates. For instance, this session will be organized focusing on advanced cluster and periodic approaches for electronic structure, state-of-the-art Density Functional Theories (DFTs) for solid-state and gas phase chemistry, atomic basis sets and effective core potentials for the simulations of heavy elements embedded in molecular frameworks.
- A half-day session dealing with the development of new approaches, codes and modeling strategies.
- A half-day session devoted to Molecular Dynamics methodologies for the simulation of reactivity of small molecular entities or atoms (e.g. heavy metal centers) trapped on adsorbing sites or vacancies of molecular frameworks. Classical, semi-classical and quantum approaches will be discussed.
- 2 half-days session on the efficient multi-scale models to predict the dynamic behavior of the active species in their real environment (e.g. micronized particles, nanoparticles, active molecules adsorbed in microporous carbon, crystalline solids, nanotubes etc.).

The main challenge in the accurate simulation of molecular systems embedded in solid macroscopic environments is the setup of a reliable procedure to transfer simulations at the nanometric scale to larger length scales. This requires the development of specific models where an interplay and expertise of different scientific communities and specialists (molecular and quantum mechanics modelers, spectroscopists, solid state physicist and engineers) is needed. Therefore, the goal of the present workshop is to fill the gap between these communities and create fruitful and long-standing joint collaborations.

C. Participants and invited speakers

The speaker list (30 minutes + 10 minutes discussion) includes former students and early careers colleagues as well as distinguished members of today's community.

This workshop is organized by Dr. Roberto Linguerri (theoretical chemist) and Dr. Nicolas Hautière (Responsible for the RG5 project at IFSTTAR, U. Gustave Eiffel)

The List of participants may include
Dr. Roberto Linguerri, U. Gustave Eiffel, France
Pr. Majdi Hochlaf, U. Gustave Eiffel, France
Dr. Nicolas Hautière, U. Gustave Eiffel, France
Pr. Gilberte Chambaud, U. Gustave Eiffel, France
Dr. Sonja Grubisic, U. Belgrade, Serbia
Dr. Rahama Dahmani, U. Tunis, Tunisia
Pr, Claro Ignacio Sainz-Díaz, Universidad de Granada, Armilla, Spain
Pr. Dezso Horvath, University of Szeged, Hungary
Pr. Francesca Mocci, University of Cagliari, Italy
Dr. Rita Prosmiti, CSIC, Spain
Pr. Miljan Dašić, Czech Technical University, Czech Republic
Dr. Julien Waytens, U. Gustave Eiffel, France
Dr. Michel André, U. Gustave Eiffel, France
Dr. Céline Villa, U. Gustave Eiffel, France
Dr. Emmanuel Chailleux, IFSTTAR MAST/MIT, France
Dr. Alexandre de Bernardinis, U. Paris Saclay, France
Dr. Bérengère Lebental, Ecole Polytechnique – U. Gustave Eiffel, France

Several other communities expressed their interest to join this event. Let's cite, for instance
Dr. Edouard Audit, Maison de la Simulation
Dr. Matthias Scheffler, Fritz Haber Institute of the Max Planck Society

Ongoing discussions are undertaken with the PIs of the EoCoE and NOMAD European projects, who are also interested to join.

D. Financial support

We request a 3k€ financial support from CECAM-FR-MOSER.

The overall provisional budget is as follows:

Expected expenses: 8 k€

- accommodation for 10 speakers: 3 k€
- grants for 10 PhD students and postdoctoral fellows: 3 k€ `
- lunches for all 30 participants during the 2 days of the workshop: 1 k€
- coffee breaks: 0.5 k€
- social dinner: 1.5 k€

Funding requests: 8 k€

- U. Gustave Eiffel: 5 k€
- CECAM-FR-MOSER: 3k€