Forschergruppe 877

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Investigation of organic-inorganic materials by MD and QM/MM simulations

Hybrid materials are solid compounds based on the association of an inorganic matrix and of an organic species. Those materials exhibit specific properties that can be modulated depending on the choice of the organic guest molecule (often a dye) and on the porous, inert and mechanically stable solid host matrix (often silica). Such hybrid materials are used in air decontamination [1], in biological and environmental sensors, in non-linear optics, as pigments [2] …

   The properties of the hybrid materials come from the subtle interactions between the organic and inorganic entities. Although fluorescence spectroscopy down to single molecule level as well as fluorescence confocal microscopy are very powerful techniques, a complementary tool to investigate hybrid materials at the nanometric scale is molecular dynamics (MD) and a deeper analysis can be performed using QM/MM simulations where the organic molecule is described at the quantum chemical level in the presence of the inorganic matrix represented by classical models. This talk will present the development of such a QM/MM code based on two well-known parallel codes (SIESTA [3] for QM and DL_POLY [4] for MM) and on a fast TDDFT calculation [5] of the electronic spectra. The development of the QM/MM code is supported by the NOSSI ANR project "New Tools for the Simulations of Surfaces and Interfaces".

   However, in this classical or QM/MM approach, the use of MD simulations lies on empirical force fields describing both organic and inorganic entities and also crossed interactions. Those latter raise a key problem, most simulations facing two difficulties:
      - Assumption of rigid frameworks ignoring then the flexilibity issue or,
      - poor representation of the inorganic-organic interactions because of the incompatibility
       of the large partial charges in oxide models ($q_{Si} > 2e$) [6] with those in typical molecular
       force fields ($q < 0.5e$).

Therefore, we provide an improved force field for silicas [7], able to describe their structure and their dynamics and compatible with the molecular interactions in organic systems. The force field describes both dense silicas like α-quartz or α-cristobalite and a microporous silica like silicalite, including its low affinity for water. We have also developed force fields for modelling the hydroxyl groups of silica surfaces and for other Mg- and Al-based oxides. These force fields allow us to investigate hybrid materials and will also be presented in this talk.

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