UNIVERSITÀ DI SIENA 1240 | DIPARTIMENTO DI BIOTECNOLOGIE, CHIMICA E FARMACIA — DBCF

Seminar Announcement

September 4th at 11:00 am – Aula 24

Polo Universitario di San Miniato

(Online: https://meet.google.com/kpy-vvok-dci)

Towards a Realistic Modeling of Complex Systems: a Multiscale Perspective

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The theoretical description of large molecular systems in the condensed phase at a high level of accuracy is particularly challenging, due to the large number of degrees of freedom (both electronic and nuclear) that must be properly accounted for. Such a chemical complexity typically arises in molecular systems in solution or interacting with a biological matrix, and it is even more pronounced when they are adsorbed on metal nanostructures supporting plasmon excitations – the physical mechanism underlying surface-enhanced spectroscopies, such as Surface-Enhanced Raman Scattering (SERS). From a theoretical perspective, these systems can be addressed within a unified framework based on the partitioning of the total system into smaller, interacting subsystems, with specific focus on the target molecular system of interest, leading to the so-called focused models [1-3].

In this talk, I will present and discuss the recent developments in focused methods rooted in multiscale quantum mechanical (QM)/classical methodologies specifically designed to accurately describe complex molecular systems interacting with an external environment [3-5]. Various applications, ranging from chromophores in solution [3] or embedded in a biological matrix [4] to molecular systems interacting with plasmonic substrates [5], will be discussed to illustrate the reliability and robustness of the approaches, also through direct comparison with experimental data [3-9]. Finally, I will outline some future perspectives on emerging complex phenomena that call for novel theoretical approaches.

References

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The course is valid for the acquisition of credits as part of the doctoral programmes in Chemical and Pharmaceutical Sciences

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