Laboratoire SRSMC
Equipe Théorie-Modélisation-Simulation
Université de Lorraine & CNRS

Dr. Marco Marazzi
Boulevard des Aiguillettes
Vandoeuvre-lès-Nancy, Nancy, France

Tel +33 - 383 68 43 72
Fax +33 – 383 68 43 71
marco.marazzi@univ-lorraine.fr

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Motivation Letter

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Efficient computer codes are a present requirement in the area of photo-dynamics. Indeed, computational studies concerning the excited-state dynamics of different systems are making possible the comparison with time-resolved spectroscopy methods. Nevertheless, new codes are needed to investigate the photo-dynamics of complex molecular systems.

With this aim, we propose a collaboration between the group of Prof. Dr. Antonio Monari (Université de Lorraine, Nancy, France) and the group of Prof. Dr. Leticia González (University of Vienna, Vienna, Austria). More in detail, the group in Nancy (including the postdoctoral project of the applicant) is specialized in the multi-scale modelling of DNA photo-sensitization through organic molecules; on the other hand, the group in Vienna has developed the SHARC code, a software package devoted to the excited-state dynamics of molecules.

Within the MOLIM COST action, both mentioned professors are part of Working Group 2 – Time-Resolved Method Developments, being Prof. González an MC member and Prof. Monari a non-MC member.

Even though different interfaces to the SHARC code do exist, no one can deal with complex environments required to simulate DNA photo-sensitization. We therefore propose the development of the SHARC-DALTON interface, since the DALTON code is presently used in Nancy to calculate bio-molecular properties by Time Dependent – Density Functional Theory (TD-DFT). This will constitute a novelty for the SHARC code and will allow the study of the benzophenone-mediated DNA photo-sensitization, a topic of interest in the group of Prof. Monari.

With best regards,

(Dr. Marco Marazzi).