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"Una manera de hacer Europa"
AGENCIA ESTATAL DE INVESTIGACIÓN
PID2021-127554NA-I00
ICMOL INSTITUTO DE CIENCIA MOLECULAR
VNIVERSITAT DE VALÈNCIA

Junior Postdoctoral Position

Project: Computational photochemistry with multiscale methods

Research area: Theoretical and computational chemistry, photochemistry

Place: Institute for Molecular Science (ICMol), University of Valencia, Spain

Conditions: 1 year with possibility of extension according to accomplished objectives. Gross salary around 26.800 € / year.

Starting date: June-July 2023.

Application deadline: Interested candidates should contact Dr. Antonio Francés (antonio.frances@uv.es) and Prof. Daniel Roca (daniel.roca@uv.es) **before May 26th**. Candidates should include their CVs (including complete contact information for two references) and a motivation letter describing why the candidate should be considered for this position.

Project description: Computational photochemistry aims to simulate molecular photoresponses of interest in technology, biology, and medicine. Advances in surface-hopping non-adiabatic molecular dynamics allow the characterization of the main photochemical decay paths taking place in the sub-picosecond scale, including both non-reactive and photoreactive pathways.

Many photochemical phenomena require the use of highly correlated multiconfigurational quantum chemistry methods and accurate determinations of the couplings between states (non-adiabatic couplings, spin-orbit couplings). Whereas surface-hopping methods have been successfully implemented for molecular models in the gas phase, the influence of complex environments such as biological macromolecules or air-water interfaces remains mainly unexplored and demands efforts in the use and validation of multiscale QM/MM schemes coupled with excited-state dynamics.

This post-doctoral project is thus devoted to set up surface-hopping dynamics studies of molecular systems embedded in complex environments by testing recent implementations of these methods. The molecules of interest will fall in the fields of emergent anticancer phototherapies, atmospheric chemistry, photobiology, and/or technology.

Requirements:

- PhD in **theoretical and computational chemistry**.
- PhD defense: **later than July 2019**.
- Strong background in **multiscale** (QM/MM) dynamics.
- Good **programming skills** and Linux management.
- Fluent English (oral and written) and good communication skills.

Complementary skills:

- Background in theoretical photochemistry.
- Experience in electronic structure software and *ab initio* surface-hopping dynamics (OpenMolcas, Gaussian, Orca, Bagel, SHARC, Newton X, etc.).

Research context: The researcher will join the *Quantum Chemistry of the Excited State of Valencia (@qcexval)* group (http://qcexval.uv.es), which accumulates a dilated experience in the **quantum-chemical characterization** of photophysical and photochemical processes with relevance for technology, biology, and medicine. The researcher will be integrated within the Molecular Science Institute (ICMol) of the University of Valencia, a multidisciplinary research institute committed with excellence (María de Maeztu Excellence Unit).

Relevant bibliography related to this project:

1. Photochemical and thermochemical pathways to S_2 and polysulfur formation in the atmosphere of Venus, A. Francés-Monerris,* J. Carmona-García, T. Trabelsi, A. Saiz-Lopez, J. R. Lyons,* J. S. Francisco,* D. Roca-Sanjuán,* ***Nat. Commun.*** 2022, *13*, 4425.
2. Light-Induced On/Off Switching of the Surfactant Character of the o-Cobaltabis (dicarbollide) Anion with No Covalent Bond Alteration, A. M. A. Abdelgawwad, J. A. M. Xavier, D. Roca-Sanjuán, C. Viñas, F. Teixidor,* A. Francés-Monerris,* ***Angew. Chem. Int. Ed.*** 2021, *60*, 25753-25757.
3. Photochemistry and Non-adiabatic Photodynamics of the HOSO Radical, J. Carmona-Garcia, A. Frances-Monerris, C. A. Cuevas, T. Trabelsi, A. Saiz-Lopez, J. S. Francisco,* D. Roca-Sanjuan,* ***J. Am. Chem. Soc.*** 2021, *143*, 10836-10841.
4. Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates, A. Francés-Monerris,* M. Lineros-Rosa, M. A. Miranda, V. Lhiaubet-Vallet, A. Monari,* ***Chem. Commun.*** 2020, *56*, 4404-4407.
5. Photodissociation mechanisms of major Hg(II) species in the atmospheric chemical cycle of mercury, A. Francés-Monerris, J. Carmona-García, U. Acuña, J. Dávalos, C. Cuevas, D. Kinnison, J. Francisco, A. Saiz-Lopez*, D. Roca-Sanjuán*, ***Angew. Chem. Int. Ed.*** 2020, *59*, 7605-7610.