Postdoctoral Position

Project: Computational modelling of supramolecular polymers

Research area: Theoretical and computational chemistry and supramolecular chemistry

Conditions: 1 year with possibility of extension according to accomplished objectives. Gross salary between 27.900 and 36.650 € / year depending on the postdoc experience.

Starting date: Sept-Dec 2023.

Application deadline: Interested candidates should contact Dr. Juan Aragó (juan.arago@uv.es) and Prof. Enrique Ortí (enrique.orti@uv.es) **before July 10th**. 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: Supramolecular polymers are a type of polymers whose monomeric building blocks are molecular units held together *via* noncovalent interactions. Supramolecular polymers have attracted a great deal of attention as multifunctional materials for biomedical and optoelectronic applications. However, the large size of the supramolecular polymers and the relevance of solvent effects in the self-assembly make the computational modelling of these polymers very challenging. This project aims at developing multi-scaled computational protocols to describe accurately the mechanism of supramolecular polymerization growth (pathway complexity, supramolecular polymorph transitions, co-polymerization process, …) as well as the chiral transfer and amplification phenomena that occur in these polymers. In addition to the theoretical aspects, the post-doctoral research fellow will be involved in stimulating collaborations with experimental groups where, in general, an atomistic picture of the supramolecular organization is missing and the theoretical simulations are highly valuable.

Key requirements:

- PhD in **theoretical and computational** chemistry.
- Experience in large-scale **molecular dynamics** simulations.
- Familiar with **self-assembly** processes.
- Knowledge in **programming** and Linux management.
- Fluent **English** (oral and written) and good communication skills.

Research context: The researcher will join the *Molecular Materials Theoretical Chemistry* group (MolMatTC), which accumulates a dilated experience in the **computational characterization** of electroactive molecular materials with relevance for (opto)electronic applications. The researcher will be integrated within the Molecular Science Institute (ICMol) of the University of Valencia, which is a multidisciplinary research institute committed with excellence (distinguished as a Maria de Maeztu research unit).

Relevant bibliography related to this project:

1. Thermodynamics of the Self-Assembly of N-Annulated Perylene Bisimides in Water. Disentangling the Enthalpic and Entropic Contributions *Org. Chem. Front.* **2023***, 10,* 1959. https://doi.org/10.1039/D3QO00111C
2. Thermoreversible Polymorph Transitions in Supramolecular Polymers of Hydrogen-Bonded Squaramides *Angew. Chem. Int. Ed.* **2022**, *61*, e202213345. https://doi.org/10.1002/ange.202213345
3. Influence of the Z/E Isomerism on the Pathway Complexity of a Squaramide-Based Macrocycle *Small* **2021**, *17*, 2006133. https://doi.org/10.1002/smll.202006133
4. Distance Matters: Biasing Mechanism, Transfer of Asymmetry, and Stereomutation in N-Annulated Perylene Bisimide Supramolecular Polymers *J. Am. Chem. Soc.* **2021**, *143*, 13281. https://doi.org/10.1021/jacs.1c06125
5. Dual-Mode Chiral Self-Assembly of Cone-Shaped Subphthalocyanine Aromatics *J. Am. Chem. Soc.* **2020**, *142*, 21017. https://doi.org/10.1021/jacs.0c07291