

## PhD in Computational Chemistry

A fully-funded 4-yr PhD position in computational chemistry is available at the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona in the frame of the project "Emergence of optical and redox properties in biochemical systems", under the supervision of Prof. Lluís Blancafort. Expected starting date is January 2024. The position is funded as an FPI fellowship from the Spanish Ministry of Science and Innovation (MICINN), project ref. PID2022-138062NB-I00.

The PhD project title is "DEVELOPMENT AND VALIDATION OF A THEORETICAL MELANIN PLATFORM".

We are looking for candidates willing to work collaboratively. Good English skills, a background in theoretical/computational chemistry or physics and some programming skills will be a plus. Candidates need a master's degree in chemistry, physics or related subjects, and have to register at the School of Doctoral Studies of the University of Girona by the start of the contract, *ie* the requirements to register need to be met by the start of the fellowship.

The *Excited States and Non-Adiabatic Processes* group of Lluís Blancafort (<http://iqcc.udg.edu/wordpress/portfolio/lluís-blancafort/>) is part of the IQCC. The IQCC (<http://iqcc.udg.edu>) has around 100 members and offers an international research environment at the forefront of computational chemistry and catalysis.

Interested candidates please send a CV including undergraduate and Master's grades, a motivation letter and the names of two referees to [lluís.blancafort@udg.edu](mailto:lluís.blancafort@udg.edu).

For further inquiries do not hesitate to contact Lluís Blancafort at this e-mail address.

Related references:

- "Indole-5,6-quinones display hallmark properties of eumelanin" Wang, X.; (...); Blancafort, L.; Kohler, B.; Lumb, J.-P. *Nat. Chem.* **2023**, *15*, 787-793.
- "Fingerprint-based deep neural networks can model thermodynamic and optical properties of eumelanin DHI dimers" Bosch, D.; Wang, J.; Blancafort, L. *Chem. Sci.* **2022**, *13*, 8942.
- "Stability and Optical Absorption of a Comprehensive Virtual Library of Minimal Eumelanin Oligomer Models" Wang, J.; Blancafort, L. *Angew. Chem. Int. Ed.* **2021**, *60*, 18800-18809.