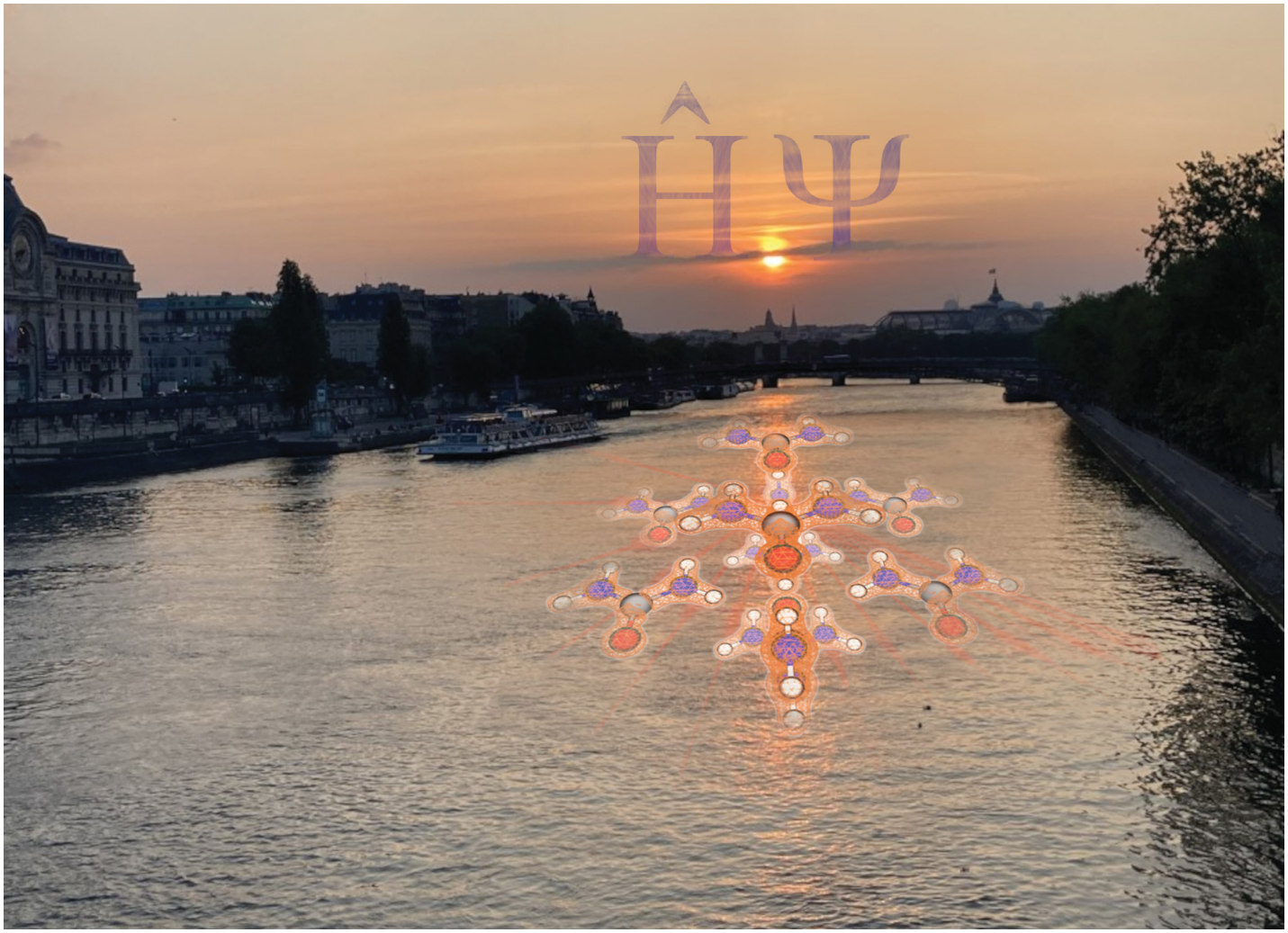

Showcasing research from the group of Prof. Julia Contreras-García at Sorbonne University, Paris.

How do density functionals affect the Hirshfeld atom refinement?

This work analyzes the effect of varying some physical quantities, such as the mixture of Hartree–Fock exchange which are usually adjusted Density Functional Theory calculations, on the refinement parameters obtained from the Hirshfeld atom refinement. The observed trends are opposite to those normally seen from geometry optimizations. Thus, it may be the case that the development of density functionals or basis sets suitable for quantum crystallography should take a different path than those fitted for quantum chemistry computations.

As featured in:

See Bruno Landeros-Rivera, Julia Contreras-García *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 12702.

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