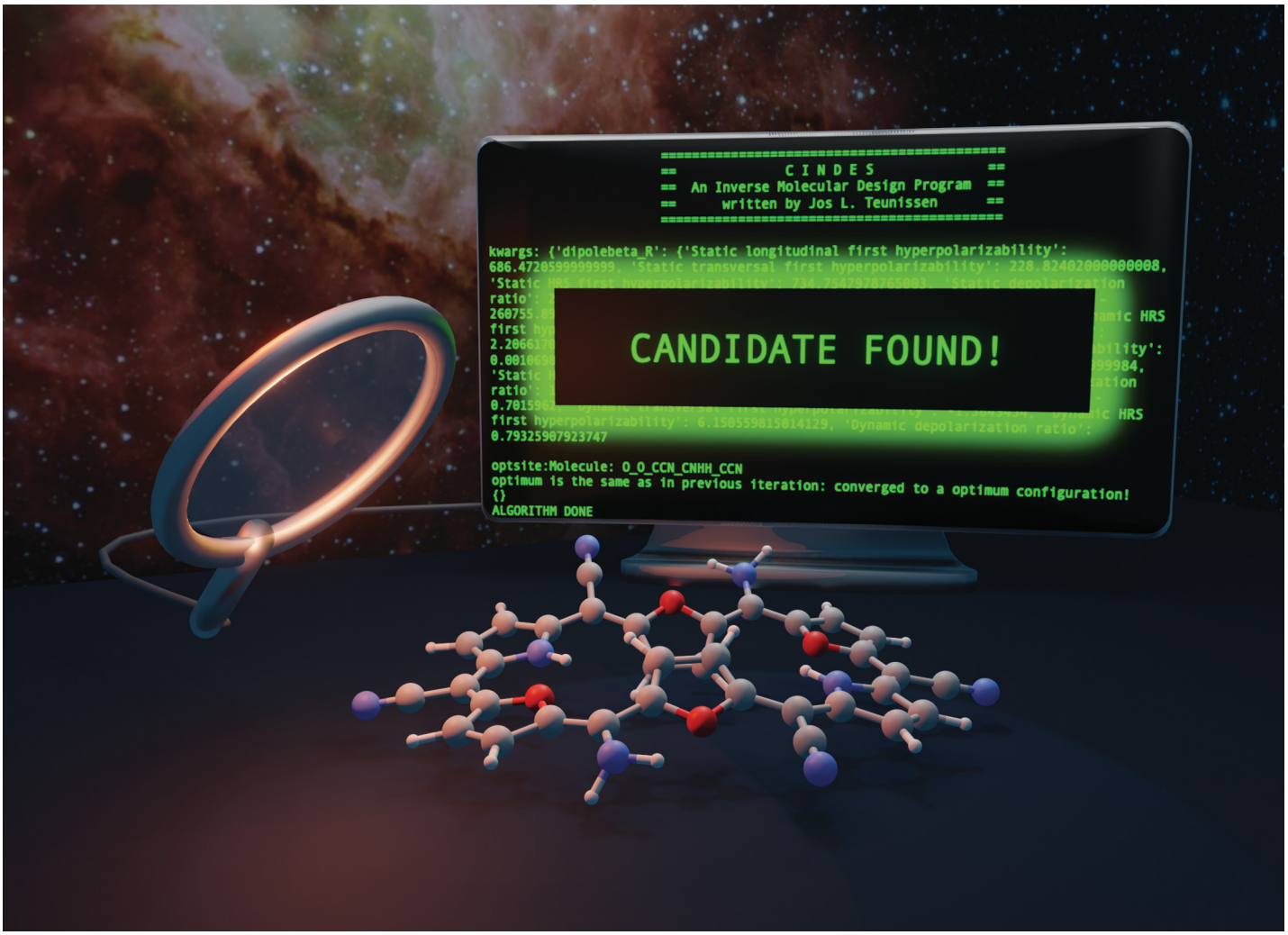

Showcasing research from the Quantum Chemistry Group at Vrije Universiteit Brussel, Belgium

Designing hexaphyrins for high-potential NLO switches: the synergy of core-modifications and *meso*-substitutions

This study showcases the application of inverse design to traverse the chemical compound space in search of nonlinear optical switches based on functionalized hexaphyrins. With the inverse algorithm, we generated a database of 277 functionalization patterns towards high-potential switches. We demonstrated that combinations of *meso*-substitutions and core-modifications significantly enhance the NLO contrast. After a thorough database analysis, we derived several design rules for obtaining efficient NLO hexaphyrin-based switches that could help to understand the contributing factors in tuning their NLO contrast.

As featured in:

See Mercedes Alonso, Freija De Vleeschouwer *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 17128.

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