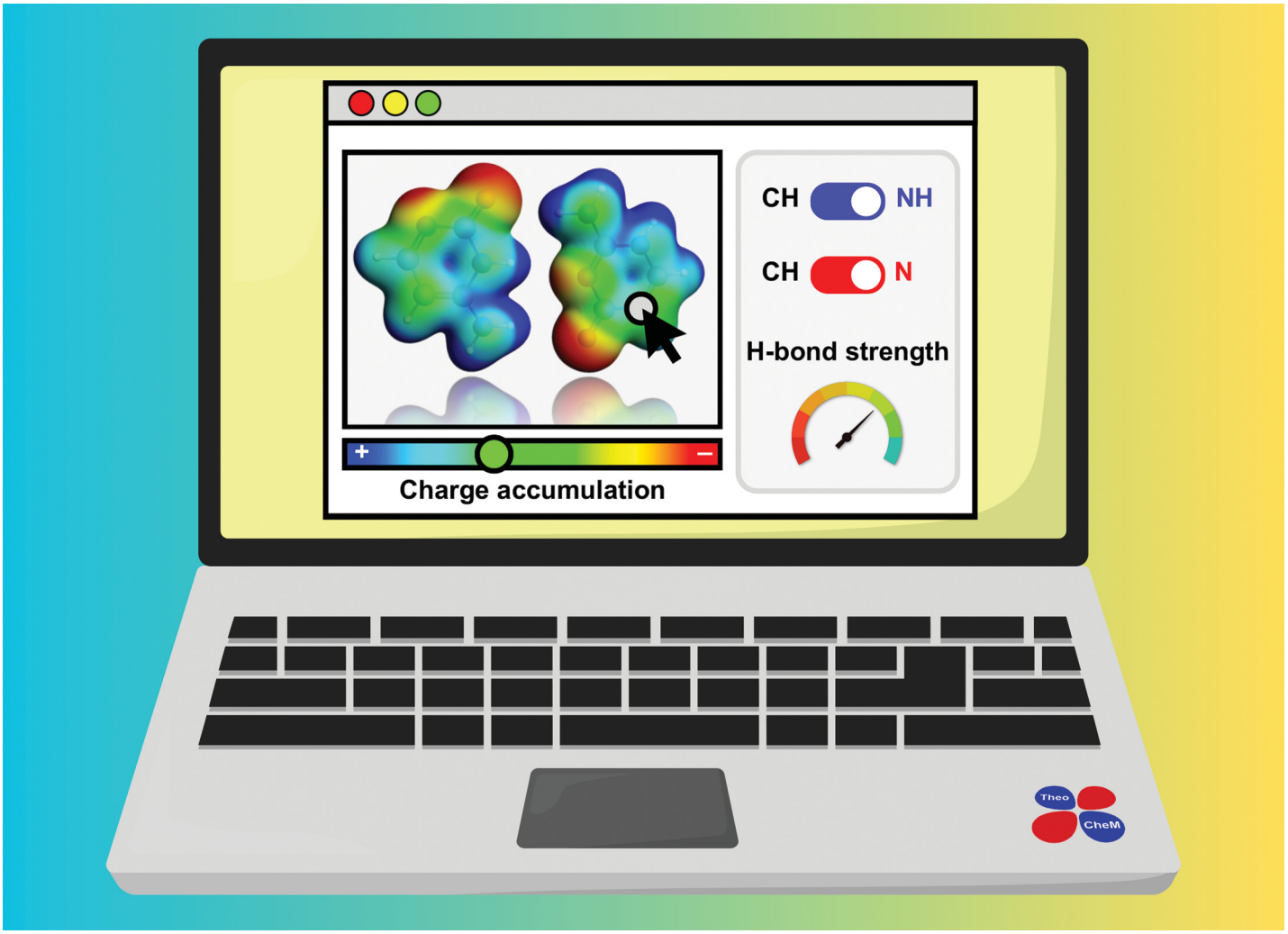

Showcasing research from the group of Professor Célia Fonseca Guerra at the Vrije Universiteit Amsterdam, The Netherlands

Multiple hydrogen-bonded dimers: are only the frontier atoms relevant?

The Fonseca Guerra Group studies the nature and strength of weak chemical interactions in biological and supramolecular self-assembled systems through state-of-the-art quantum-chemical methods and analyses. This work shows that non-frontier atom exchanges in hydrogen-bonded aromatic dimers can induce significant interaction energy changes (up to 6.5 kcal mol^{-1}). It is demonstrated that the relative hydrogen-bond strengths of these *N*-edited base pair isosteres, which cannot be explained from the front atoms, follow from the charge accumulation in the monomers.

As featured in:

See Célia Fonseca Guerra *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 11306.

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