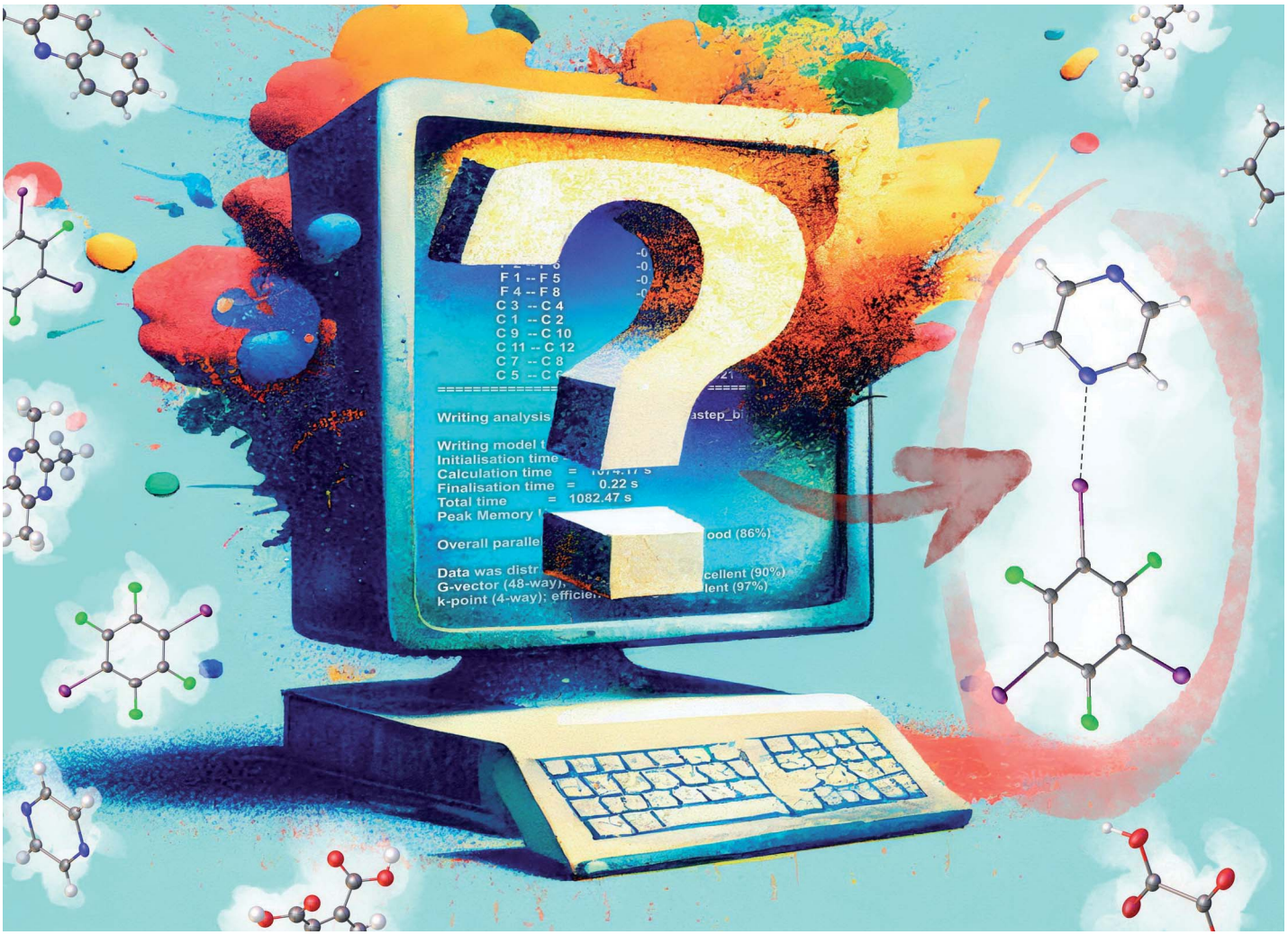
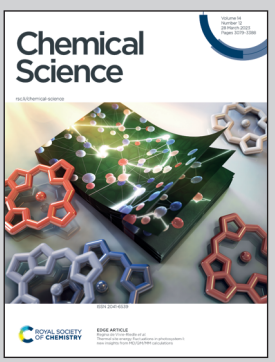


Showcasing research from Professor Arhangelskis' laboratory, Faculty of Chemistry, University of Warsaw, Poland.

Computational evaluation of halogen-bonded cocrystals enables prediction of their mechanochemical interconversion reactions

We present the combined use of periodic density-functional theory (DFT) calculations and dissolution calorimetry measurements to predict the thermodynamic feasibility of mechanochemical interconversions for molecular crystals containing halogen bonding interactions. By calculating the relative lattice stability of multiple cocrystals, differing in either donor or acceptor component, we are able to systematically predict which coformer exchange reactions will occur under experimental conditions, and which ones will not. This approach allows us to design mechanochemical reactions of cocrystals and foresee their outcomes before performing any experimental work.

As featured in:



See Mihails Arhangelskis *et al.*, *Chem. Sci.*, 2023, **14**, 3140.

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