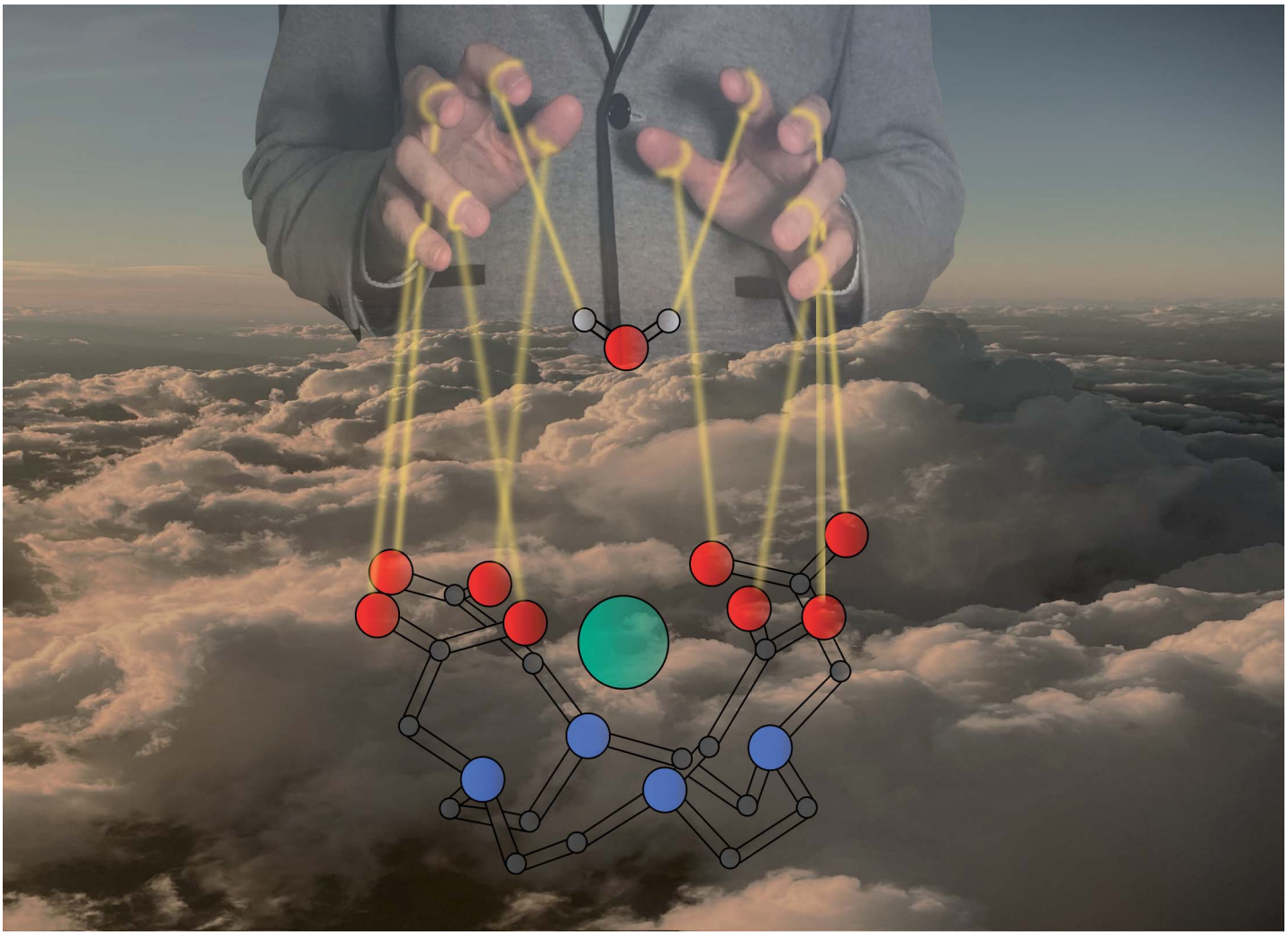
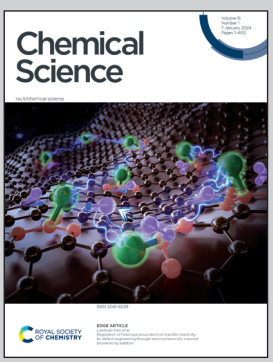


Showcasing research from laboratories of: i) Professor Mauro Perfetti, Department of Chemistry, University of Florence, Italy; ii) Professor Matteo Briganti, Department of Chemistry, University of Florence, Italy; iii) Professor Annie Powell, Institute of Inorganic Chemistry and Institute of Nanotechnology, Karlsruhe Institute of Technology; iv) Professor Jesper Blixen, Department of Chemistry, University of Copenhagen.

LnDOTA puppeteering: removing the water molecule and imposing tetragonal symmetry

The water molecule was excluded from the lanthanide coordination sphere of LnDOTA complexes (Ln = Tb to Yb) without altering the chemical structure of the DOTA ligand. Our complexes are designed to be geometrically tetragonal: strict crystallographic symmetry is achieved by exploiting solution ionic strength and solid state packing. Our combined experimental and theoretical approach has been used to unravel the electronic structure and magnetic anisotropy of the complexes. This investigation proves that the water molecule is a key factor in defining the magnetic anisotropy.

As featured in:



See Matteo Briganti, Jesper Bendix, Mauro Perfetti *et al.*, *Chem. Sci.*, 2024, **15**, 113.

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