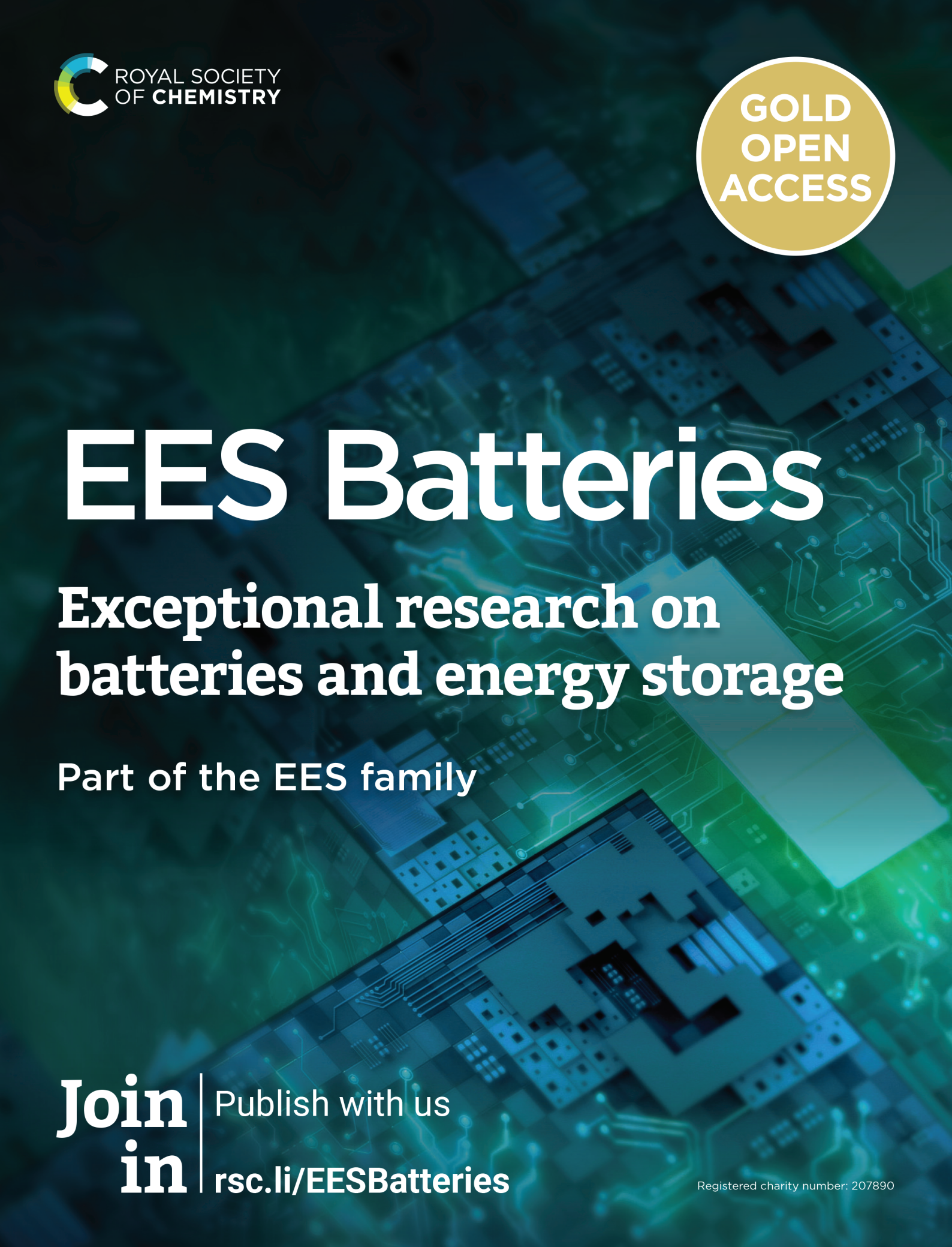
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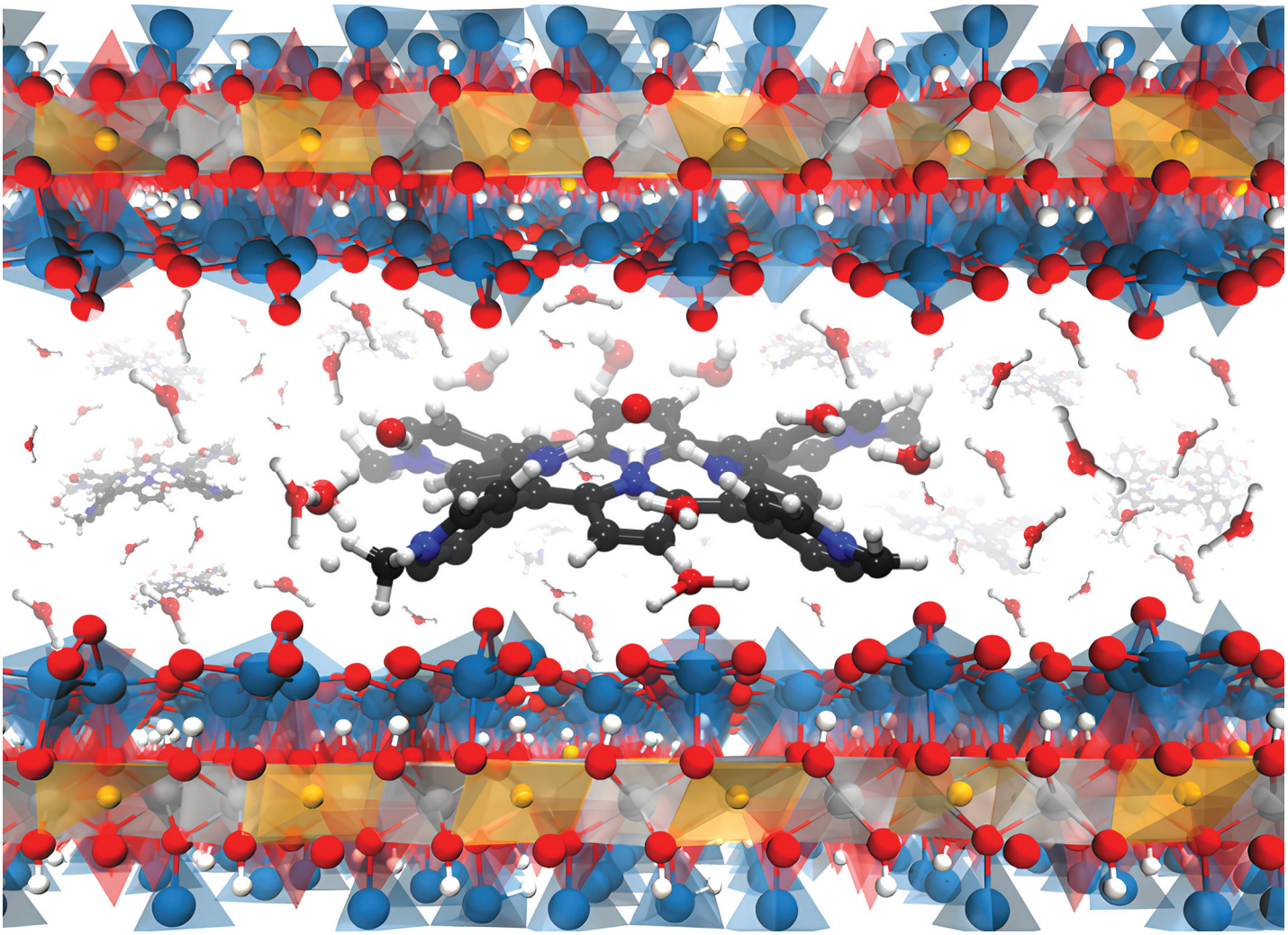

Showcasing research from Professor Helena Petrilli's group, Department of Materials Physics, Institute of Physics, São Paulo University, Brazil.

Shape-responsive host–guest chemistry: metal-free tetracationic porphyrin nonplanarity promoted by clay mineral interactions assessed by theoretical simulations

DFT calculations indicate that interactions with montmorillonite lead to conformational changes in porphyrins, such as twisting of the macrocycle and rotation of the peripheral substituents. These changes increase basicity and facilitate the abstraction of protons from intercalated water. This highlights the significant role of clay microenvironments in modifying the properties of porphyrins.

As featured in:

See Vera Regina Leopoldo Constantino, Helena Maria Petrilli *et al.*, *Dalton Trans.*, 2025, **54**, 2271.

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