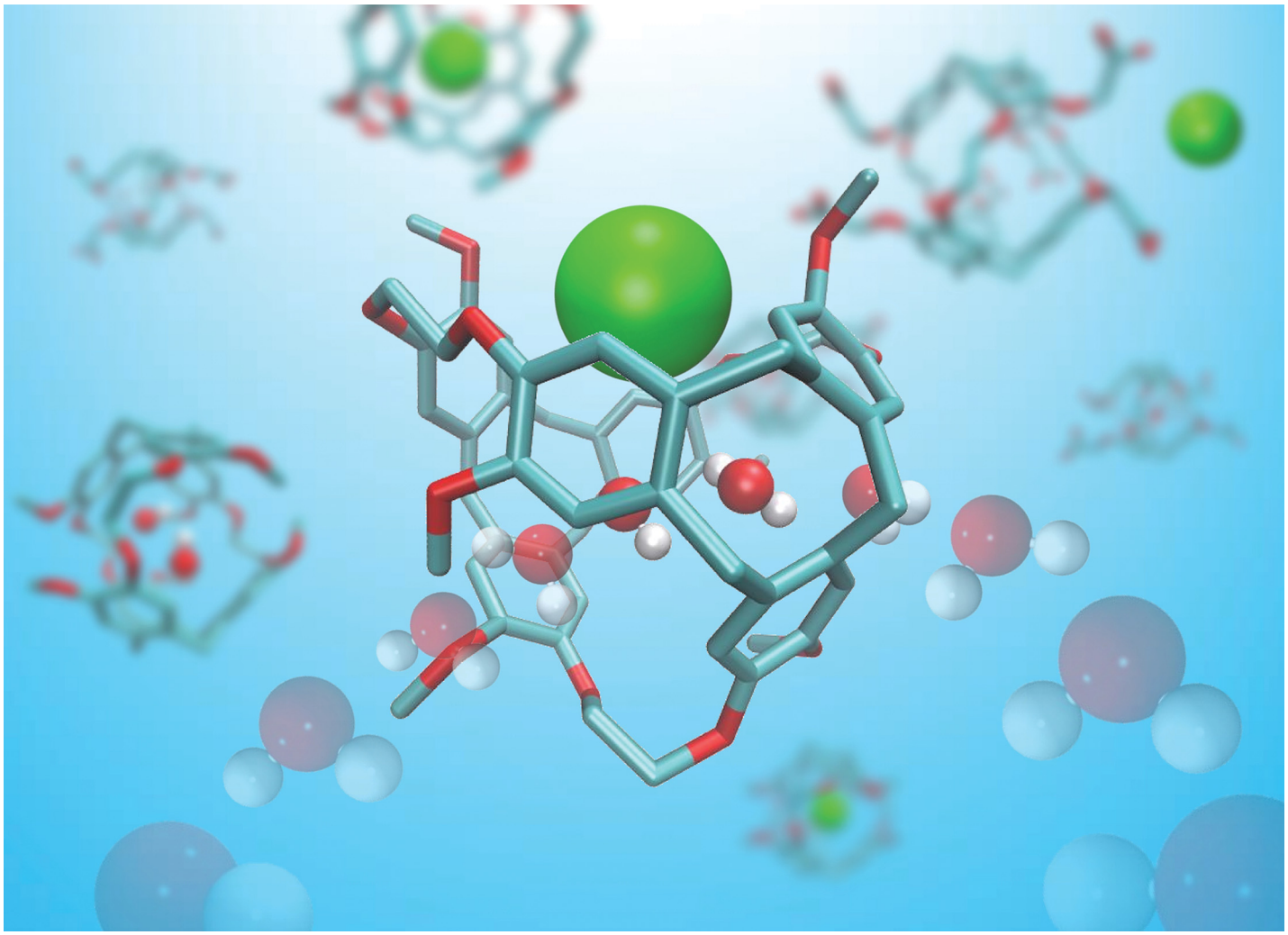
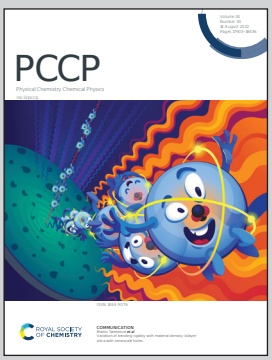


Showcasing research from the NMR Research Unit, University of Oulu, Finland.

Energetics and exchange of xenon and water in a prototypic cryptophane-A biosensor structure

In this work, state-of-the-art semiempirical molecular dynamics and metadynamics simulation methods are applied for the first time to the energetics and dissociation mechanism of a Xe atom between a Xe NMR biosensor cage and aqueous solution. The Xe dissociation pathways, the gating mechanism associated with the cage opening and the role of the in-out exchange of water molecules in initiating the Xe dissociation, are established. This provides detailed microscopic insight into this process that is crucial for the *in vivo* applications of Xe biosensors.

As featured in:



See Perttu Hilla and J uha Vaara, *Phys. Chem. Chem. Phys.*, 2022, 24, 17946.

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