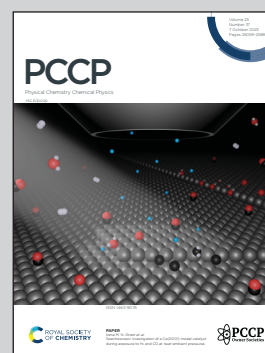


Showcasing research from the Molecular Simulation Group of Prof. Longhua Yang at the School of Pharmaceutical Sciences, Zhengzhou University, Henan, China

New insights into the proton pumping mechanism of ba_3 cytochrome c oxidase: the functions of key residues and water

This work explored the functions of a series of key residues and water for the proton pumping mechanism of ba_3 -type cytochrome c oxidase using molecular dynamics simulations and quantum cluster models calculations. Our research provides a more profound understanding of the proton pumping mechanism, which is also helpful for the determination of proton pumping states in experiment.

As featured in:



See Longhua Yang *et al.*,
Phys. Chem. Chem. Phys.,
2023, **25**, 25105.