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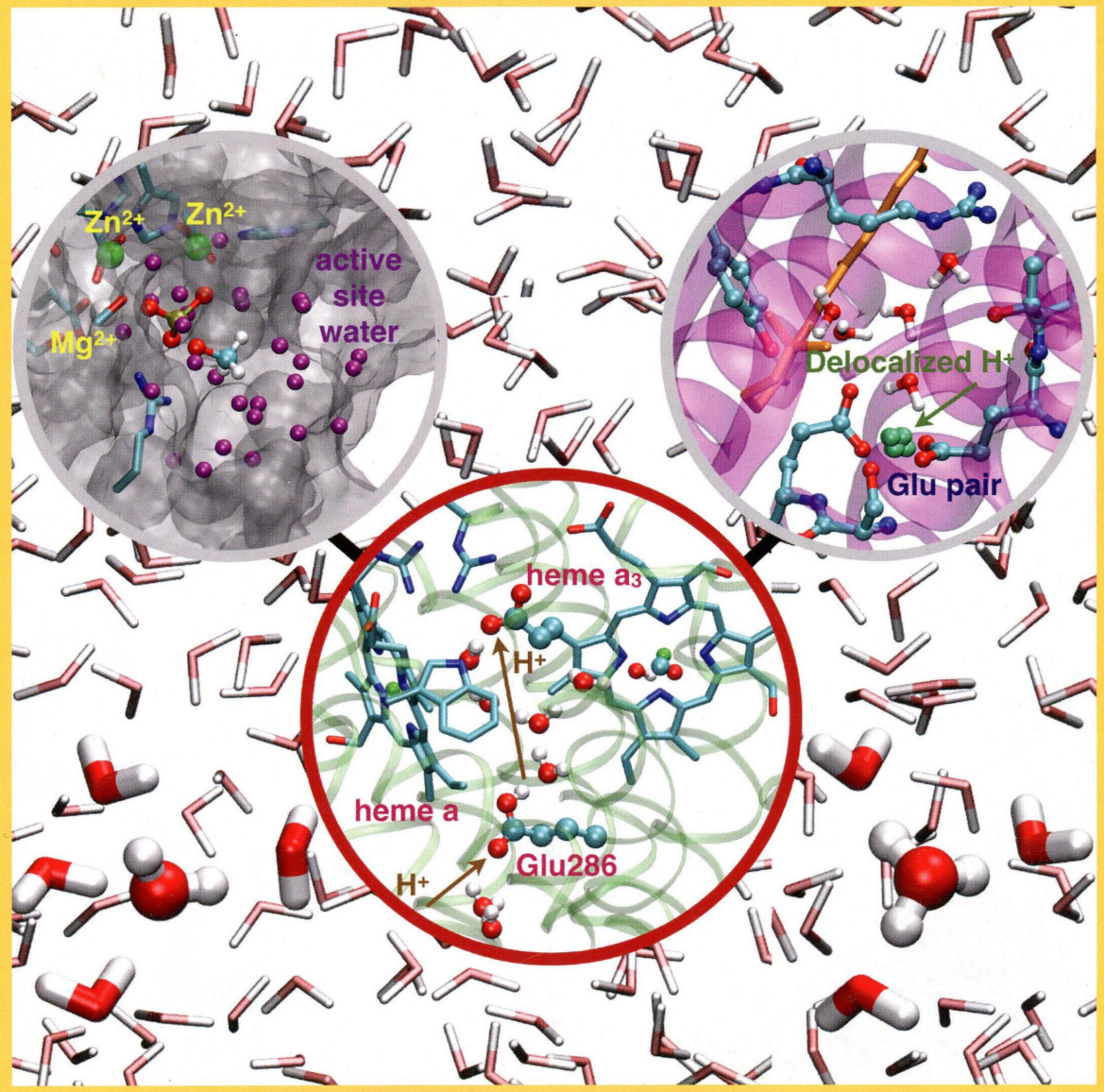

Water and the Hydrated Proton in Different Environments: Bulk Water and Protein Interiors (see page 5A)

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ON THE COVER: Examples that illustrate recent applications of the DFTB3/MM model where a quantum mechanical description of water proved essential: (clockwise starting from the upper left corner) catalytic specificity and promiscuity in alkaline phosphatase are modulated in part by solvent molecules accessible to the active site; the proton storage site in bacteriorhodopsin involves a proton delocalized between amino acid side chains that are solvated by active site water; proton transfers in cytochrome c oxidase proceed through water wire; and a neutral glutamate near a hydrophobic cavity. See Goyal, P.; Qian, H.-J.; Irle, S.; Lu, X.; Roston, D.; Mori, T.; Elstner, M.; Cui, Q. Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models. *J. Phys. Chem. B* **2014**, *118* (38), 11007−11027, DOI: 10.1021/jp503372v.

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