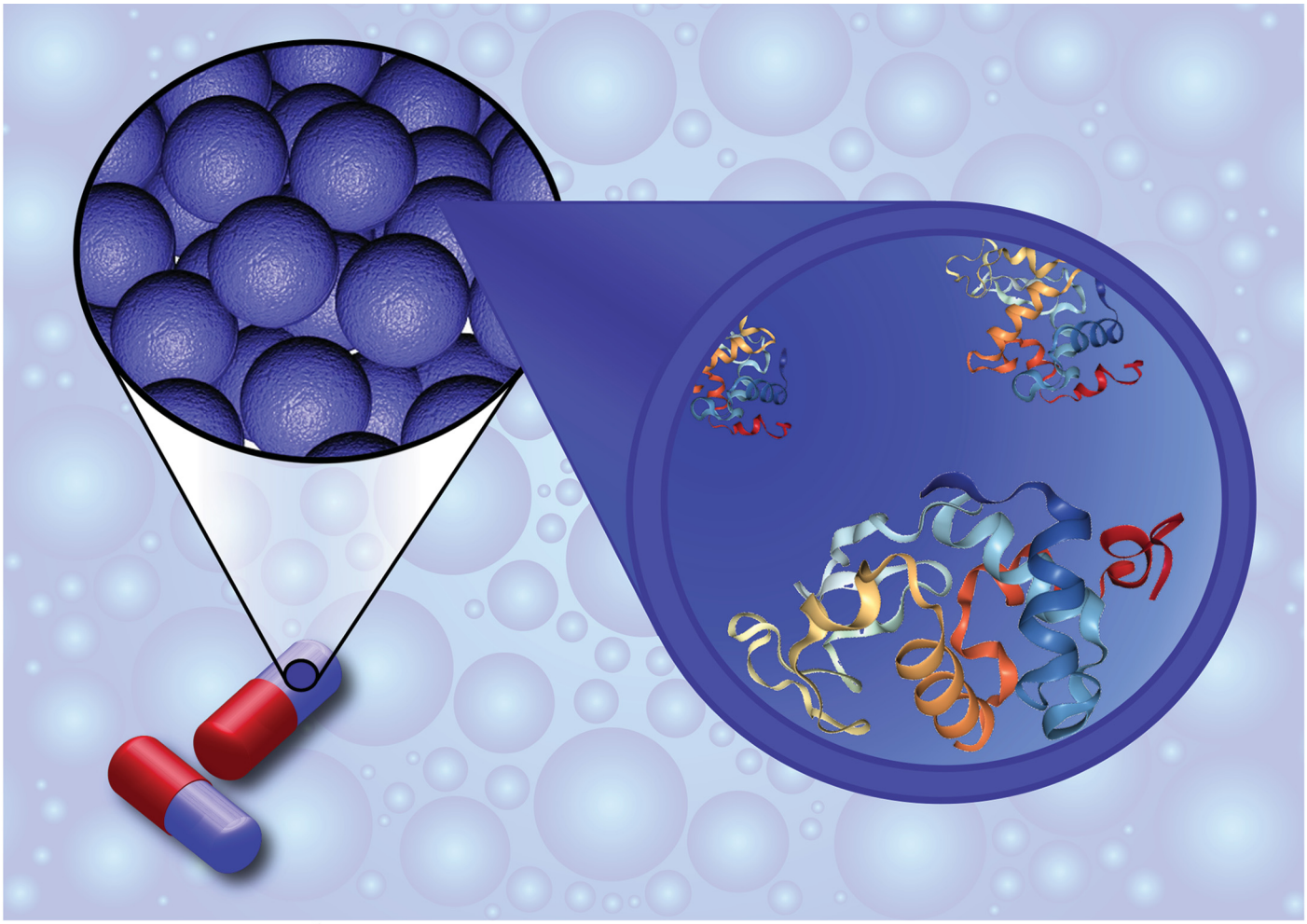


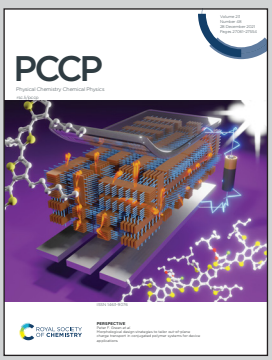
Image source: pixabay.com/Mol* Viewer[1] by using PDB ID 3wun (DOI:10.2210/pdb3wun/pdb) from rcsb.org.
1 D. Sehnal, S. Bittrich, M. Deshpande, R. Svobodová, K. Berka, V. Bazgier, S. Velankar, S. K. Burley, J. Koča, A. S. Rose, *Nucleic Acids Res.*, 2021, **49**, W431–W437.

Showcasing research from the groups of Prof. Sidney de Carvalho at Sao Paulo State University, Brazil, and Prof. Ralf Metzler at Potsdam University, Germany.

Adsorption of lysozyme into a charged confining pore

This work investigates the adsorption of hen egg-white lysozyme into charged pores *via* computational approaches. The results of Monte Carlo simulations show that the protein adsorbs into charged pores in two pH-dependent orientations. The electrostatic potential at the amino-acid residues closer to the pore surface affects their protonation degree, thereby favoring the adsorption. The results presented in this study provide valuable information for applications, such as the protein and drug delivery by nanoparticles of mesoporous silica.

As featured in:



See Sidney J. de Carvalho *et al.*, *Phys. Chem. Chem. Phys.*, 2021, **23**, 27195.

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