SFB 1078

Protonation Dynamics in Protein Function

Mon, **Nov. 8th** 2021

15:15 – 16:15

Freie Universität Berlin

Hörsaal B

Colloquium

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Noncovalent Interactions Using Crystal Structure Data and Quantum Chemical Calculations

Crystal structures in the Cambridge Structural Databank (CSD) were analyzed to determine and characterize molecular interactions, their frequencies, and preferred geometries. Quantum chemical calculations were performed to evaluate the energies of these interactions. With this methodology, our group recognized different types of new noncovalent interactions: stacking interactions involving (i) planar metal-chelate rings, (ii) organic aromatic rings at large offsets, and (iii) CH-pi interactions of chelate rings. The calculated energies showed that the stacking of metal-chelate rings is stronger than stacking between two benzene molecules. Studies of interactions of coordinated ligands indicate stronger noncovalent interactions than interactions of non-coordinated molecules.

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