Quantum refinement:
Working closely with experiment

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Experimental structures are widely used in computational studies. They can be used as starting geometries for calculating properties, or to validate computational results. However, for macromolecules, experimental results are itself in part determined by theory. Often molecular mechanics force fields are employed. Quantum chemical tools are used sometimes, but only as a separated part in the process.

Quantum refinement helps to determine structures from experimental raw data by fully integrating quantum mechanics into the refinement protocol. It can be applied to various experimental techniques, e.g., NMR, EXAFS, and X-ray crystallography. As a result, such refined structures are a compromise between theory and experiment, making them more realistic. In this presentation, examples of a few systems are given with a more detailed discussion on BLUF (sensor of blue light using flavin adenine dinucleotide) domain-containing proteins.