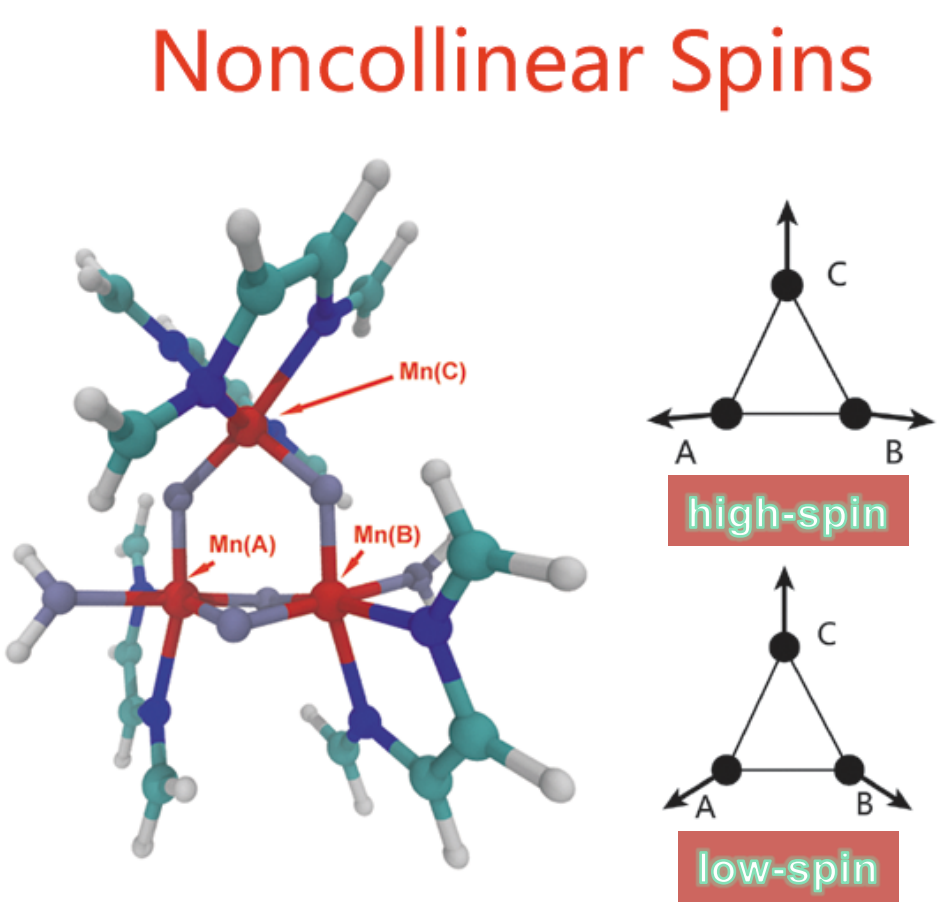
Noncollinear Spins Revealed in Biomimetic Mn_3 Core of OEC in PSII

- The oxygen-evolving complex (OEC) of Photosystem II plays a key role in the photoenzymatic oxidation of H_2O to O_2, which is the key reaction in the earth's solar energy cycle.
- Convential DFT methods constrain electron spins to be either up or down (collinear), and cannot describe the Mn_3 oxomanganese core of the OEC self-consistently.
- Noncollinear DFT reveals that the spin on each Mn is in a different direction, and self-consistent calculations give good agreement with experiments.
- Noncollinear spins provide new, more powerful descriptions of many complexes in transition metal chemistry, especially in systems with strongly coupled open-shell centers.



Luo, Rivalta, Batista, Truhlar, J. Phys. Chem. Lett. 2, 2629 (2011)