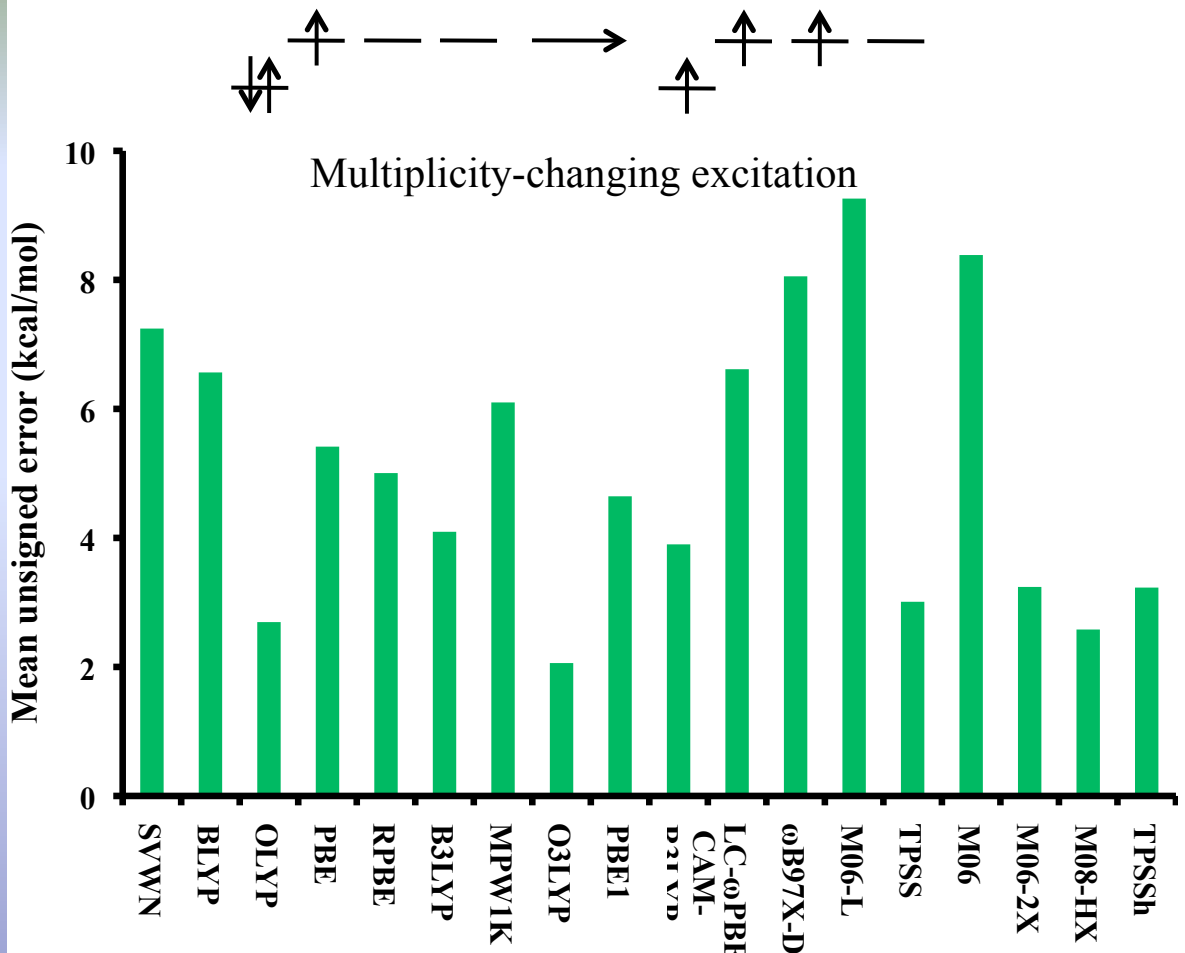
# Density Functional Study of Multiplicity-Changing Excitations

- Multiplicity-changing excitations are important for reaction mechanisms and magnetic properties.
- They are difficult for DFT since they require a balanced treatment of exchange and correlation.
- 56 density functionals were tested against experimental results; most functionals give quite large errors—exceptions being OLYP, O3LYP, and M08-HX.




*Yang, Peverati, Valero, Truhlar (U. of Minnesota), J. Chem. Phys. 135, 044118 (2011)*