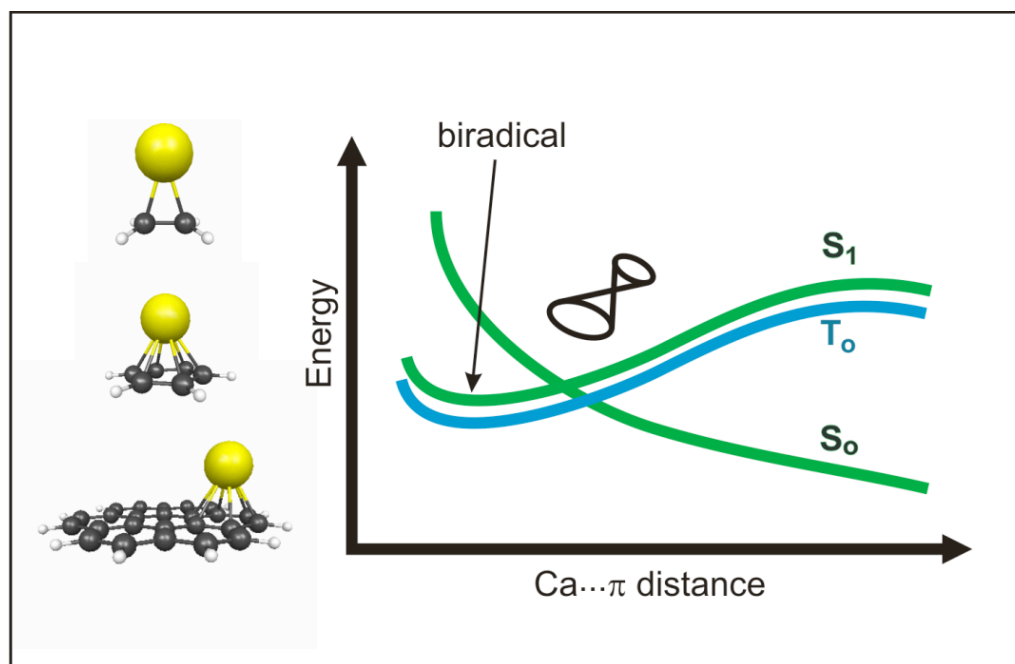


Metal-organic charge transfer

- Is mediated by conical intersections
- Can produce biradical states



“Metal-Organic Charge Transfer Can Produce Biradical States and is Mediated by Conical Intersections,” O. Tishchenko, R. Li, and D. G. Truhlar, Proceedings of the National Academy of Sciences of the United States of America **107**, 19139-19145 (2010).
[dx.doi.org/ 10.1073/pnas.1010287107](https://doi.org/10.1073/pnas.1010287107)

Metal-organic charge transfer

The interactions of metal atoms with aromatics and graphene-based materials are important for catalysis, molecular electronics, optoelectronic sensing devices. A fundamental understanding of the interfacial states of metal atoms interacting with conjugated π -systems is an essential element underlying rational molecular electronics design.

This work demonstrated that the electron transfer in metal-- π -electron systems is controlled by sequential conical intersections, and some cases produces metastable biradicals.

