

# **Pseudo Jahn-Teller Effect in photochemistry and catalytic chemistry**

**Yang Liu**

Harbin Institute of Technology, China

As the big progress in Jahn-Teller Effect field, the Pseudo Jahn-Teller Effect has become a powerful tool for understanding the origins of molecular structure for ground or excited states, predicting novel phenomenon, and showing extensive applications for molecules and solid states in the fields of photochemistry and catalysis chemistry.

In chemistry and biology fields, there is a general problem: why and how does light induce reactivity? The system becomes chemically reactive by excitation due to its polarization, and the process is called “sudden polarization”. We found the sudden polarization is induced by the PJTE in the excited state interacting with higher electronic states by taking many organic molecules as examples, and obtained a general physical picture for the photochemistry process.

We designed a diatomic catalyst which shows excellent activity for oxygen reduction reaction (ORR) with small overpotential of about 0.2V by DFT calculations. It is found that the promising catalytic activity closely relates to the asymmetric active center induced by PJTE, which could enhance the polarization for the oxygen molecule. Additionally, the asymmetric deformation of active center increases, the catalytic activity increases. The symmetry deformation degree of the active center could be an important indicator for catalytic activity.

## **References:**

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