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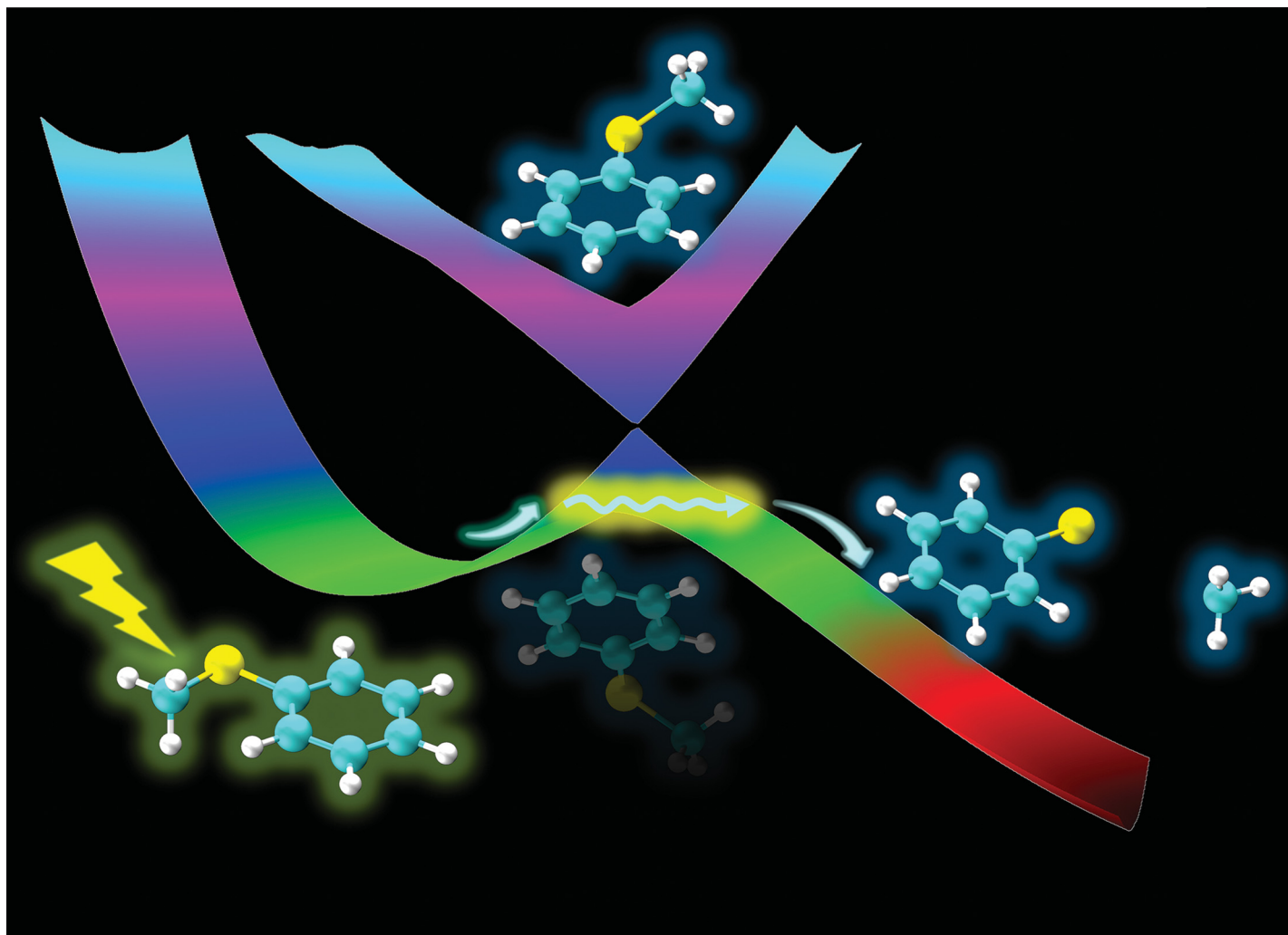
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**Showcasing research from the group of Professor Changjian Xie at Northwest University, China**

Nonadiabatic heavy atom tunneling in  ${}^1n\sigma^*$ -mediated photodissociation of thioanisole

This work investigates the  ${}^1n\sigma^*$ -mediated photodissociation dynamics of thioanisole using a quantum mechanical model based on the newly constructed diabatic potential energy matrix. Our theoretical results show that the photodissociation of thioanisole at the low-lying  $S_1({}^1\pi\pi^*)$  levels is not merely nonadiabatic but also undergoes heavy atom tunneling. Specifically, the geometric phase effect around the  $S_1/S_2$  conical intersection is found to slightly impact the lifetimes due to the weak interferences in this heavy atom tunneling process, which differs significantly from the scenario in the nonadiabatic hydrogen atom tunneling.

**As featured in:**



See Changjian Xie *et al.*,  
*Phys. Chem. Chem. Phys.*,  
2023, **25**, 18797.