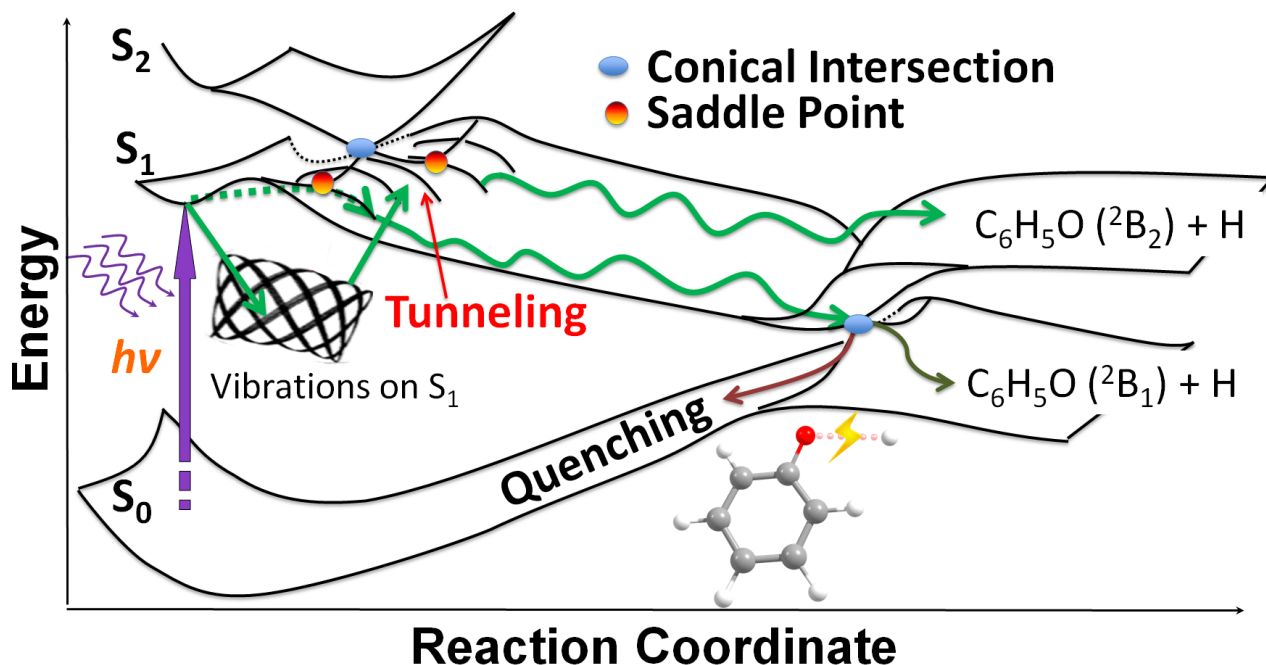


Photodissociation of Phenol: Full-Dimensional Multi-State Simulations including Tunneling



- Work combines four state-of-the-art methods in a complementary way:
- fourfold way diabaticization based on MC-QDPT
 - anchor points reactive potentials for fitting surfaces of complex systems
 - coherent switches with decay of mixing for multi-state trajectories
 - army ants tunneling

[X. Xu, J. Zheng, K. R. Yang, D. G. Truhlar, J. Am. Chem. Soc. 136, 16378 \(2016\).](#)

Work was performed at University of Minnesota.