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

Work combines four state-of-the-art methods in a complementary way:
• fourfold way diabatization 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


Work was performed at University of Minnesota.