Molecular Photogearing: Insights from Computational Studies

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The construction of molecular photogears capable of transmitting the double-bond rotary motion produced by light-driven molecular motors onto a single-bond axis is a formidable challenge in the field of artificial molecular machines [1,2]. From this perspective, it is perhaps surprising that while computational studies have made numerous contributions to the design and characterization of light-driven molecular motors [3–6], their role in advancing molecular photogearing has been comparatively marginal. In this talk, I will present two photogear designs that employ completely different working mechanisms [7,8], including one that requires no intermediary thermal steps [8], and describe assessments of their efficiency based on both static quantum chemical calculations and non-adiabatic molecular dynamics simulations.

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