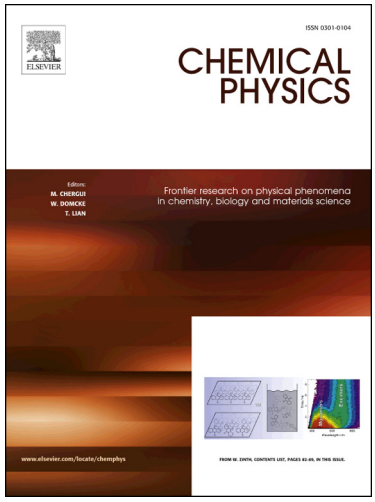

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Computational Design of a Light-Driven Imine-Based Motor with Bulky Chiral Stator

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4 Tables and 15 Figures

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Abstract

A light-driven imine-based motor with bulky chiral stator has been computationally designed by investigation of the topographical features of the potential energy surfaces. The electronically excited model imine with a *P*-helical trans form directly goes to the conical intersection (CIX) in S_1 on the downhill surface with respect to the C=N torsion. After electronic relaxation into S_0 around CIX with a double cone topography, the model imine goes to another *P*-helical cis-imine without any trap in the *M*-helical region through the C=N torsion. Thereby, the full rotary process of the imine-based motor consists of two fast photochemical steps of (*P*)-trans→(*P*)-cis and (*P*)-cis→(*P*)-trans, which is possible to realize smooth rotation by repetitive photoexcitation, unlike the previous imine-based motors with four chemical steps. In addition, the other full rotary cycle with two steps is also open, of which latter-half process of (*P*)-cis→(*P*)-trans is the slow thermal N-inversion.