The alchemy of light: computational investigation of photoswitches and photomotors

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Photochemistry holds great potential for sustainable chemistry. However, the lack of comprehensive design principles and detailed information on molecular excited-state structures hinders its full utilization. Quantum chemical simulations have emerged as indispensable tools for unraveling the intricate relationships between molecular structure and properties in photoexcited processes. Nevertheless, performing excited-state computations demands theoretical expertise and *a priori* knowledge of the photochemical properties of the system, such as spectroscopic data.

Addressing this challenge, our objective is to distill the rules and concepts governing photochemical reactions using quantum chemical data. To achieve this goal, we introduce the **S**urface **H**opping **N**ewly **I**nvented **T**raining **S**et for **E**xcited-state **L**earning (SHNITSEL) database [1], which contains computational data for various photoreactions. Specifically, we present excerpts from the database featuring sample molecules undergoing light-induced *cis/trans* isomerization (photoswitches) or directional rotation (photomotors).

[1] https://shnitsel.github.io