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Excited state, non-adiabatic dynamics of large photoswitchable molecules using a chemically transferable machine learning potential

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Light-induced chemical processes are ubiquitous in nature and have widespread technological applications. For example, the photoisomerization of azobenzene allows a drug with an azo scaffold to be activated with light. In principle, photoswitches with useful reactive properties, such as high isomerization yields, can be identified through virtual screening with reactive simulations. In practice these simulations are rarely used for screening, since they require hundreds of trajectories and expensive quantum chemical methods to account for non-adiabatic excited state effects. Here we introduce a neural network potential to accelerate such simulations for azobenzene derivatives. The model, which is based on diabatic states, is called the *diabatic artificial neural network* (DANN). The network is six orders of magnitude faster than the quantum chemistry method used for training. DANN is transferable to molecules outside the training set, predicting quantum yields for unseen species that are correlated with experiment. We use the model to virtually screen 3,100 hypothetical molecules, and identify several species with extremely high quantum yields. Our results pave the way for fast and accurate virtual screening of photoactive compounds.

Biography

Simon Axelrod received a Bachelor of Science degree in physics from Queen's University, Kingston in 2016. He received a Master of Science degree in physics in 2017 from the University of Toronto. He is currently a PhD student at Harvard University and is co-supervised at MIT.