World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:17, No:11, 2023

AI Predictive Modeling of Excited State Dynamics in OPV Materials

Authors : Pranav Gunhal., Krish Jhurani

Abstract : This study tackles the significant computational challenge of predicting excited state dynamics in organic photovoltaic (OPV) materials—a pivotal factor in the performance of solar energy solutions. Time-dependent density functional theory (TDDFT), though effective, is computationally prohibitive for larger and more complex molecules. As a solution, the research explores the application of transformer neural networks, a type of artificial intelligence (AI) model known for its superior performance in natural language processing, to predict excited state dynamics in OPV materials. The methodology involves a two-fold process. First, the transformer model is trained on an extensive dataset comprising over 10,000 TDDFT calculations of excited state dynamics from a diverse set of OPV materials. Each training example includes a molecular structure and the corresponding TDDFT-calculated excited state lifetimes and key electronic transitions. Second, the trained model is tested on a separate set of molecules, and its predictions are rigorously compared to independent TDDFT calculations. The results indicate a remarkable degree of predictive accuracy. Specifically, for a test set of 1,000 OPV materials, the transformer model predicted excited state lifetimes with a mean absolute error of 0.15 picoseconds, a negligible deviation from TDDFT-calculated values. The model also correctly identified key electronic transitions contributing to the excited state dynamics in 92% of the test cases, signifying a substantial concordance with the results obtained via conventional quantum chemistry calculations. The practical integration of the transformer model with existing quantum chemistry software was also realized, demonstrating its potential as a powerful tool in the arsenal of materials scientists and chemists. The implementation of this AI model is estimated to reduce the computational cost of predicting excited state dynamics by two orders of magnitude compared to conventional TDDFT calculations. The successful utilization of transformer neural networks to accurately predict excited state dynamics provides an efficient computational pathway for the accelerated discovery and design of new OPV materials, potentially catalyzing advancements in the realm of sustainable energy solutions.

Keywords : transformer neural networks, organic photovoltaic materials, excited state dynamics, time-dependent density functional theory, predictive modeling
Conference Title : ICAIMLC 2023 : International Conference on Artificial Intelligence and Machine Learning in Chemistry
Conference Location : Cape Town, South Africa
Conference Dates : November 06-07, 2023