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Computational screening of organic materials towards improved photovoltaic properties SHUO DAI, Dept. Physics, Oklahoma State Univ, ROBERTO OLIVARES-AMAYA, Dept. Chemistry, Princeton Univ, CARLOS AMADOR-BEDOLLA, Dept. Chemistry, UNAM, ALAN ASPURU-GUZIK, Dept. Chemistry, Harvard Univ, MARIO BORUNDA, Dept. Physics, Oklahoma State Univ — The world today faces an energy crisis that is an obstruction to the development of the human civilization. One of the most promising solutions is solar energy harvested by economical solar cells. Being the third generation of solar cell materials, organic photovoltaic (OPV) materials is now under active development from both theoretical and experimental points of view. In this study, we constructed a parameter to select the desired molecules based on their optical spectra performance. We applied it to investigate a large collection of potential OPV materials, which were from the CEPDB database set up by the Harvard Clean Energy Project. Time dependent density functional theory (TD-DFT) modeling was used to calculate the absorption spectra of the molecules. Then based on the parameter, we screened out the top performing molecules for their potential OPV usage and suggested experimental efforts toward their synthesis. In addition, from those molecules, we summarized the functional groups that provided molecules certain spectrum capability. It is hoped that useful information could be mined out to provide hints to molecular design of OPV materials.

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