

Abstract Submitted  
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**Computational assessment of organic photovoltaic candidate compounds** MARIO BORUNDA, SHUO DAI, Oklahoma State University, ROBERTO OLIVARES-AMAYA, Princeton University, CARLOS AMADOR-BEDOLLA, UNAM, ALAN ASPURU-GUZI, Harvard University — Organic photovoltaic (OPV) cells are emerging as a possible renewable alternative to petroleum based resources and are needed to meet our growing demand for energy. Although not as efficient as silicon based cells, OPV cells have as an advantage that their manufacturing cost is potentially lower. The Harvard Clean Energy Project, using a cheminformatic approach of pattern recognition and machine learning strategies, has ranked a molecular library of more than 2.6 million candidate compounds based on their performance as possible OPV materials. Here, we present a ranking of the top 1000 molecules for use as photovoltaic materials based on their optical absorption properties obtained via time-dependent density functional theory. This computational search has revealed the molecular motifs shared by the set of most promising molecules.

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