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RT-TDDFT Simulations of NLO-Polymers with Tunable Energy Levels[1] FERNANDO VILA, J. J. REHR, U. of Washington — Polymer-based solar cells have attracted much attention due to their potential as cost-effective light harvesting devices. A new series of NLO-polymers has been recently developed[2] where the HOMO-LUMO gap can be tuned to maximize the light absorption overlap with the solar spectrum, thus improving their photovoltaic efficiency. With the aim of predicting such HOMO-LUMO gaps, we have developed simplified models of these polymers. These models were optimized at B3LYP/6-31G(d,p) level and their UV-Vis spectra was calculated using our RT-TDDFT approach.[3] Our results show that the absolute B3LYP HOMO-LUMO gaps follow the trend seen in the experiment, but are about 0.6 eV higher than those experimentally determined. When this systematic error, which is likely due to self-energy and local-field effects, is removed by referring the theoretical and experimental values to a single compound, the agreement between theory and experiment is remarkable.

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[2]F. Huang *et al.*, J. Am. Chem. Soc. **131**, 13886 (2009).
[3]Y. Takimoto *et al.*, J. Chem. Phys. **127**, 154114 (2007).

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