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Electronic and Optical Excitations in Perylene Diimide Derived Dye Molecules from First Principles KOPINJOL BAISHYA, SERDAR OGUT[1], University of Illinois at Chicago, ERSEN METE, Balikesir University, OGUZ GULSEREN, Bilkent University, SINASI ELLIALTIOGLU, Middle East Technical University, Turkey — Halogenated perylene diimide dyes, such as Br-PDI ($Br_2C_{24}H_8N_2O_4$) and their glycine (BrGly) and aspartine (BrAsp) derivatives are known to absorb and emit light in the visible range with high quantum yields, and have good heat and chemical stability. As such, they are promising alternatives to the expensive (Ru-based) metal-driven dye sensitizers for solar cell applications. In this talk, we present results for the electronic structures, quasiparicle gaps, and the absorption spectra of PDI-derived dye molecules BrPDI, BrGly, and BrAsp, computed within the time-dependent density functional theory as well as many body perturbation techniques such as the GW method and the solution of the Bethe-Salpeter equation. In addition to discussing our results for bare molecules, we also present our preliminary studies for the change in their electronic and optical properties when they are attached to stoichiometric and reduced rutile TiO_2 (110) surfaces.

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