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# A Simple Effective $\Delta$ SCF Method for Computing Optical Gaps in Organic Chromophores

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**Abstract:** Photoluminescence effects in organic chromophores are of significant importance and requires precise description of low lying excited states. In this communication, we put forward an alternative time-independent DFT scheme for computing lowest single-particle excitation energy, especially for singlet excited state. This adopts a recently developed “virial”-theorem based model of singlet-triplet splitting which requires a DFT calculation on closed shell ground state and a restricted open-shell triplet excited state, followed by a simple  $2e^-$  integral evaluation. This produces

vertical excitation energies in small molecules, linear and non-linear polycyclic aromatic hydrocarbon and organic dyes in comparable accuracy to the TDDFT. We also explore the functional dependency of present method with three different functionals (B3LYP, wB97X and CAM-B3LYP) for polyenes and linear acenes. A systematic comparison with literature value illustrates the validity and usefulness of the present scheme in determining optical gap with fair computational cost.