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Using the particle-hole map to analyze charge transfer excitations in molecular complexes[1] EDWARD A PLUHAR, University of Missouri - Columbia, YONGHUI LI, Tianjin University, CARSTEN A ULLRICH, University of Missouri - Columbia — The particle-hole map (PHM) is a computational tool to visualize electronic excitations (calculated using time-dependent density-functional theory), based on representations in canonic molecular orbital transition space. We have effectively demonstrated the PHMs ability to map out the origins and destinations of electrons and holes and, hence, the roles of different functional units of organic molecules during an excitation. Beyond the standard canonical representation, transformation to localized orbitals is a common technique. We analyze the PHM as a visualization tool for both canonical and localized molecular orbital representations in various inorganic and organic charge-transfer complexes.

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