A quantitative assessment of electronic transitions' charge-transfer character

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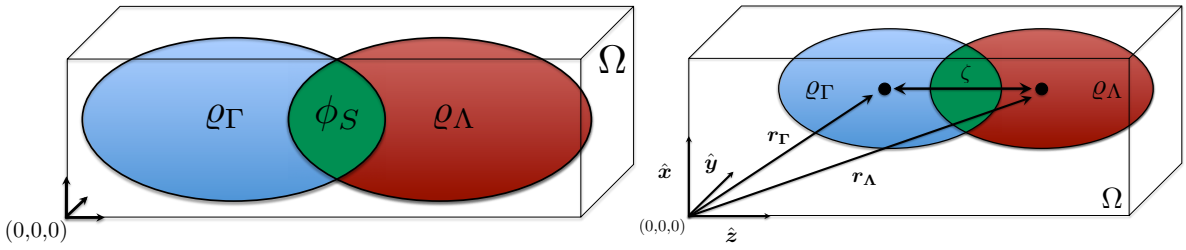
The present communication relates recent studies devoted to a topological descriptor of photoinduced electronic charge density variation, called ϕ_S. This new index consists in a quantity related to detachment and attachment densities overlap, where the detachment and attachment physically represent electronic density depletion and increment induced by light absorption. Complementarily to former approaches based on direct space charge density variation, our new method provides a simple way to evaluate the charge transfer induced by light absorption. This index can be used as a diagnostic test of exchange-correlation functionals. Furthermore, this model can lead to the evaluation of new push-pull dyes charge-transfer ability to assess their potentiality as candidates for dye-sensitized solar cells. After discussing the new ϕ_S descriptor's mathematical foundations from various perspectives (detachment/attachment densities, natural transition orbitals), its application to several types of chromophores will be exposed. Connexions and divergences will finally be drawn with formerly known indices.



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