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Photophysical properties of molecular compounds: insights from Density Functional Theory

The performances of Density Functional Theory (DFT) and Time Dependent DFT (TD-DFT) in the prediction of ground and excited state properties of molecular systems (both fully organic or containing d or f transition metals) will be reviewed by selected examples of compounds used in molecular devices with application ranging from hybrid photovoltaic cells to molecular spintronic.[1-7]

Special emphasis will be devoted to the possibility of providing a realistic description of the environmental effects (ex. solvent, absorption on a surface, encapsulation) on the overall photophysical properties of these systems by the means of theoretical methods ranging from continuum polarizable models for solvent, cluster approaches, QM/QM' or periodic calculations. Finally, a recently proposed index enabling to quantify the extent and magnitude of transferred charge associated to a charge transfer (CT) excitation [8], will be illustrated and applied to the description of CT excitations in push-pull donor-acceptor systems providing insights on its potential application for the designing and development of novel molecular materials [9].

References

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Ilaria Ciofini got her graduate degree in Chemistry at the University of Florence (Italy) in 1997 in the research group of Profs. Alessandro Bencini and Dante Gatteschi, focusing on the theoretical prediction of the magnetic properties of molecular inorganic complexes. After, she moved to join the group of Prof. Claude Daul (Univ. of Fribourg, Switzerland) for a Ph.D. in theoretical chemistry (2001) concerning the application and development of methods for the description and prediction of magnetic and electronic properties of molecular compounds. After one year postdoctoral fellow at the University of Wurzburg (Germany) in the group of Prof. Martin Kaupp and two years as CNRS associate researcher at Chimie-Paristech (Paris, France), she got a permanent CNRS position Chimie-Paristech (2004) where, from 2010, she is CNRS Research Director. Her main research interests concern the development and application of DFT methods to molecular compounds for the prediction of properties ranging from magnetic to photophysical ones.