Abstract Submitted
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Prediction of the absolute charge mobility of molecular crystals
ALESSANDRO TROISI, University of Warwick — I propose a computational protocol to predict the absolute mobility of molecular semiconductors without adjustable parameters. The system dependent parameters are computed using a combination of classical molecular dynamics simulations and quantum chemical methods. The model used to connect the computable quantities with the observable temperature dependent mobility takes into account the effects of molecular reorganization energy and the fluctuation of the transfer integral due to thermal motions. The absolute value of the hole mobility, computed for the case of rubrene, is in excellent agreement with the experiments. The possibility of using computational chemistry methods to improve the theoretical models of charge transfer will be discussed in some detail. The predictive capabilities of the model presented in this work will be further validated considering the recent THz spectroscopy measurements performed by R. van Laarhoven in Eindhoven and the results in literature on temperature dependent band structure and density of state tails.

Alessandro Troisi
University of Warwick

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