Point Charge Embedding Schemes for Excited State Processes in Molecular Organic Crystals

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ABSTRACT

Modelling excited state processes in organic molecular crystals is essential for understanding relevant applications in areas such as light-emitting solid materials and organic solar cells. In this talk, I will discuss the performance of different embedding schemes based on cluster models in comparison with periodic TDDFT, G_0W_0-BSE, and experimental data.[1,2] I will analyse the impact of using different types of point charges, including periodic (Ewald) and regular embedding schemes, on the prediction of energy gaps and absorption spectra in molecular organic crystals.[3] Additionally, I will address some challenges in the application of these techniques for describing excited states in covalently linked systems, including covalent and metal- organic frameworks (COFs and MOFs).[4] The talk will also highlight the applications of these techniques in investigating aggregation-induced emission and room temperature phosphorescence materials.[5,6]

References

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