Electrostatic embedding for solid-state excited-state calculations: an application to two-dimensional transition metal dichalcogenides

Alexandre Huguet[1], Ilaria Ciofini[1], and Frédéric Labat[1]

[1] *Chimie ParisTech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, Chemical Theory and Modelling Group, 11 rue Pierre et Marie Curie, Paris, 75005, FR, France*
alexandre.huguet@chimieparistech.psl.eu

ABSTRACT

Due to the high computational cost still associated to excited-state calculations at the solid-state, electrostatic embedding schemes combined to TD-DFT appear as an attractive alternative for the accurate modeling of the photophysical properties of materials at low computational cost [1]. In particular, approaches devised to reproduce the exact Coulomb potential of an infinite periodic crystal with a large array of fitted point charges, such as the Self-Consistent Ewald (SC-Ewald) approach, have been proposed and successfully applied to various complex systems and processes [2, 1], and later extended to materials with reduced periodicities [3].

In this contribution, we present application of such an approach to the modeling of the UV-Vis. simulation of a series of two-dimensional transition metal dichalcogenides materials with reduced periodicities, in view of their importance in optoelectronic applications.

References

[1] Turelli, M.; Ciofini, I.; Wang, Q.; Ottochian, A.; Labat, F.; Adamo, C. Organic compounds for solid state luminescence enhancement/aggregation induced emission: a theoretical perspective. *Phys. Chem. Chem. Phys.* **2023**, *25*, 17769-17786.

[2] Wilbraham, L.; Labat, F.; Ciofini, I. Electrostatic Embedding To Model the Impact of Environment on Photophysical Properties of Molecular Crystals: A Self-Consistent Charge Adjustment Procedure. *J. Chem. Theory Comput.*, **2016**, *12*, 3316–3324.

[3] Luise, D.; Wilbraham, L.; Labat, F.; Ciofini, I. Modeling UV-Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. *J. Comput. Chem.* **2021**, *42*, 1212-1224.