Computational predictions of Pt(II)-based crystal structures and their emissions

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Phosphorescent platinum(II) complexes are well known for their diverse photophysical and spectroscopic properties, as evidenced by their use in bioimaging, photocatalysis or, most often, in phosphorescent light-emitting diodes (OLEDs) with varying degrees of success. [1] The goal of this work is to help implement a computational protocol that can predict the crystal structure that a Pt(II) complex will create and further predict structure's influence on a crystal's emissive properties (which remains challenging with contemporary research methods).

Our research assesses the ability of cheap computational methods to predict recently synthesized Pt(II)-based crystal structures. Semi-empirical methods were used to prescreen all possible intermolecular contacts of selected Pt(II) systems and used to build energetically competitive crystal structures. Subsequent DFT calculations were then used to ascertain if the semiempirical methods could predict the correct crystal structure and describe how the most stable intermolecular motifs manifest within them.

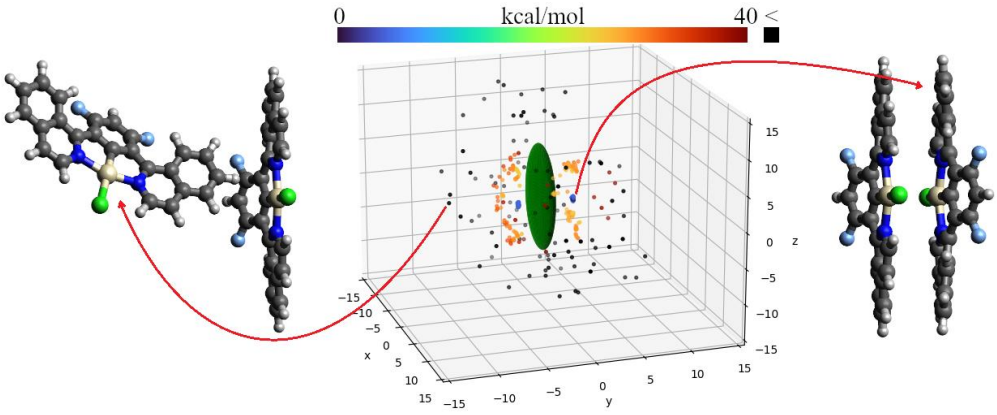

Figure 1: Schematic representation of possible dimer binding energies and symbolic geometries.

References

[1] Li, K et al. Highly phosphorescent platinum(II) emitters: photophysics, materials and biological applications. *Chem. Sci.*, **2016**, *7*, 1653-1673.