Theoretical design and prediction of phosphorescent emissive materials based on halogen bonding interactions and experimental verification of their properties

Design of new materials is a permanent process deeply engrained in the technological and economic advancement of humankind. What matters, though, is not just which materials shall we develop, but also *how* do we do that. By and large, till now, new materials are developed in research laboratories via so-called experimental screenings, where a variety of compounds is treated under different experimental conditions, till a material satisfying the desired properties is found. This is costly and time consuming. Recently, however, more and more focus is given to computational methods, as an alternative to traditional experimental screening. Computational design has multiple advantages: it releases research scientists from performing laborious experimental trials and allows them to focus on more creative tasks, saves on costs of conducting experiments, reduces energy consumption and chemical waste. At the same time, computational studies help not only predict, but also better understand the properties of materials and mechanisms of their action. With the advancement of increasingly accurate methods of computational simulations, accompanied by the growth in available computing power, a shift towards computational materials design is both expected and highly desired.

Research in our group focuses on the development of advanced methods for computational materials design. In this project we are exploring the effects of so-called halogen bonding interactions towards generation of new type of phosphorescent optical materials. Halogen bonding is a highly unusual interaction, that brings together molecules containing halogen bond donors (typically iodine or bromine atoms) and acceptor sites (oxygen, nitrogen, sulphur atoms, aromatic rings) together, allowing to form crystals containing multiple different molecules in close proximity, thus yielding materials with properties different from those of individual molecular components analyzed separately. One highly exciting effect enabled by halogen bonding is the ability to induce so-called phosphorescence emission of organic molecules. Unlike more commonly occurring fluorescence, phosphorescence is characterized by significantly longer lifetimes (think of luminous watches with dials glowing in the dark) and possible changes in emission color. Of course, real-life applications of phosphorescence are far more diverse, with particular highlights including biological imaging of inner body tissues, dyes for the detection of fingerprints and illicit substances, as well as anti-counterfeit protection of banknotes, just to name a few.

The aim of this project is to develop computational methods that explain the ability of molecules to form halogen bonding interactions in solid state, predict how these molecules “prefer” to arrange into crystal structures and finally simulate the optical properties of resulting materials, that is to estimate the ability of said material to produce phosphorescent emission and predict its’ color. At each step of the calculations we will perform experiments to verify the accuracy of our predictions and modify the computational methods as needed. In the end we shall learn how to predict structures and optical properties of halogen-bonded crystals entirely computationally, so that only structures posed to have interesting properties will be synthesized experimentally.