Modeling electroluminescent materials using a new family of electronic structure methods

Abstract for the general public

Photochemistry is a modern branch of chemistry that, broadly speaking, studies the absorption and emission of light by molecules. Optoelectronics is an interdisciplinary branch of science that merges photochemistry, materials science and other fields. One of the fundamental challenges in optoelectronics is design and study of organic light-emitting diodes (OLEDs) which has great academic and industrial interest.

Light-emitting diode (LED) is a device which emits light in response to an electric current. A special type of such device is an organic light-emitting diode (OLED) where the electroluminescent layer comprises an organic compound responsible for the emission of light. The applications of OLEDs are widespread and nowadays they are found in numerous pieces of modern technology, such as mobile phones and digital cameras, among others. They have numerous advantages important for the consumers in terms of convenience and aesthetics. Indeed, displays based of OLEDs can be manufactured to be thinner and lighter than the liquid crystal display (LCD), have higher contrast ratio and deeper black levels.

In this project we will study a class of chemical compounds which are derivatives of the molecule called heptazine. These compounds have a rare property – their first excited singlet electronic state has a lower energy than the first triplet excited state. This enables to harvest energy from both states in the emission of light. At the same time, heptazine-based materials are experimentally accessible, relatively cheap and stable within the relevant temperature range. Due to this attributes, they are good candidates for application in the next-generation of OLEDs.

We plan to study the potential of the heptazine-based compounds as OLEDs electroluminescent materials by using novel electronic structure methods. Our results will shed light on importance of various effects on the efficiency and practicality of employing heptazine derivatives as electroluminescent organic compounds. This will help in further experimental studies and refinement of these materials.