“Light” it be, or a computational insight into the optical materials properties

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The presentation will deal with the applications of the first-principles and/or semi-empirical models to the description and explanation of properties of various optical materials.

The following representative examples will be shown and discussed:

i) modification of the ternary chalcopyrite composition and its effects on the optical and electronic properties of the solar cell materials, e.g. $CuGa_{1-x}Al_xS_2$ and $CuAl(Se_{1-x}S_x)_2$. In particular, it was shown that it is possible to enhance their absorption properties in the visible spectral range by varying the second cation concentration.

ii) consistent studies of the transition metal and rare earth ions in a free state and in crystals using the ab initio and crystal field models. The performed calculations of the Slater integrals and spin-orbit constant values for the whole groups of the 3*d*, 4*d*, 5*d*, 4*f*, 5*f* ions in different oxidation states allowed to find certain linear trends linking the parameters of the electrostatic and spin-orbit interactions, thus considerably decreasing the number of independent parameters int he free ion’s Hamiltonian. By combining the crystal field and ab initio calculating techniques, complete energy level schemes of the doped compounds that include the impurity ion’s energy levels superimposed onto the host’s band structure were obtained.

iii) systematic analysis of the optical properties of the Mn^{4+} - containing red phopshors for white LEDs applications. It has been shown that the variation of the Mn^{4+} emission wavelengths is related to the degree of nephelauxetic effect experienced by the impurity ions. The Mn^{4+} emission is shifted towards longer wavelengths in more covalent oxide hosts and towards shorter wavelengths in more ionic fluoride materials. An empirical model has been developed to describe the observed experimental spectroscopic data. Detailed consideration of the structural arrangements of ligands around the Mn^{4+} ions (including the chemical bond lengths and angles between the chemical bonds) helps in understanding spectroscopic trends across the large groups of phosphor materials. Several practical advices on how to engineer the Mn^{4+} red emission properties are suggested.