Interesting Theoretical Problems in Luminescence from Solids

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Luminescence in solids, particularly large gap ionic crystals doped with optical active ions, provides a unique area of research for testing components of the quantum theory of solids. While research in luminescence was originally driven by phenomenological models based on elements of ad hoc models derived from quantum theory and experiment, rigorous applications of first-principles theory of the electronic structure of solids to validate components of these qualitative models are still lagging behind experiment. This is mainly because of the complexity of the underlying electronic excitations and emission processes of many electron systems, and partly because of the difficulty of developing computational procedures that can mimic these processes with full theoretical rigor.

During the last few decades, significant progress has been made in computational methods of electronic structures of solids. These methods have been applied, sometimes very successfully, to explore luminescence mechanisms. However, there are many luminescence processes described in the literature for which the nature of the electronic states involved in the excitation and emission processes have not been well understood, and therefore cannot be easily constructed. Some of these processes will be discussed in this presentation. It will be shown how these processes could be rigorously addressed using state-of-the-art quantum mechanical computational methods.