How to make “good” phosphors via first-principles modelling

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Abstract

This course is designed to consist of three 45 min. lectures and is tailored for Ph.D. students and interested researchers specializing in the field of luminescence physics. The primary objective of this course is to equip participants with the knowledge and skills needed to design novel luminescent materials doped with lanthanide, transition-metal, and ns^2-type ions using a first-principles modeling approach. The course will commence with a discussion of conventional defect spectroscopy based on crystal-field theory, illuminating how we comprehend luminescence within the framework of quantum physics. We will delve into the intricacies of first-principles methodology for modeling defects in solid materials, offering in-depth explanations and showcasing several successful examples of its application. Furthermore, the course will explore the cutting-edge topic of metal halide perovskites to underscore the validity of our theoretical framework and its synergistic relationship with experimental findings. The lecture topics are outlined as follows:

Lecture 1. Spectroscopy of lanthanide, transition-metal and ns^2-type ions in solids: Fundamental concepts and their crystal-field representation

Lecture 2. First-principles calculations for intrinsic and extrinsic defects in solids: Methodology and case studies

Lecture 3. Extending our understanding to metal halide perovskites: A unified physics perspective on both defects and host materials.