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Computational methods in their application to optical materials

Fast development of computer facilities and quantum chemical calculations made computational materials science be a very important tool in modern research aimed at design, development and understanding of novel functional materials with enhanced performance.

This special issue is focused on applications of various computational methods to the description of physical properties of optical materials. Density Functional Theory (DFT)-based computational techniques, semiempirical crystal field models, machine learning and other tools used for explanation of experimental results, deeper understanding of optical materials properties and smart search for new materials with advanced characteristics are discussed in the special issue papers. All authors of these selected papers are well-known scientists who made solid contributions to their respective fields of research.

Wide range of presented methods and approaches, together with broad scope of the considered materials and phenomena (phosphors, optical thermometers, radiative and non-radiative transitions) will make this collection of papers an interesting and valuable source of scientific information for an audience ranging from postgraduate students to experienced researchers.

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