专题：A 激发态过程、元激发和非线性光学；B 稀土和过渡族元素的发光

Calculations of the spectroscopic properties of transition metal and rare earth ions in optical materials

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Transition metal and rare earth ions are widely used in various optical devices and materials such as solid state lasers, phosphors for lighting, phosphorescent sensors, solar energy conversion materials etc. They have rich energy level schemes, which arise from their unfilled 3d and 4f electron shells. In the present work an overview of spectroscopic properties of the transition metal and rare earth ions in a free state and in crystals will be given. Several trends between the main parameters describing the energy levels of the ions with unfilled d electron shell will be highlighted[1-3]. Applications of several different approaches (e.g. crystal field theory, DFT-based computational techniques, configurational coordinate model etc) to various optical materials with these impurity ions will be discussed, with special emphasis on how to identify location of the impurity ions energy levels in the host band gap. It will be shown that by combining the crystal field theory and ab initio methods of electronic structure calculations it is possible to build up the complete energy level scheme of a doped crystal, which includes the host's electronic band structure and impurity ion energy levels superimposed onto it [4-6]. All calculated results will be compared with corresponding experimental data; agreement (or the reasons for disagreement) between the theory and experiment will be discussed.

关键词：Crystal-field(晶场); DFT(密度泛函理论); transition metal ions; rare earth ions

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