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Theory of Luminescent Emission in a Nanocrystal Doped by Co^{2+}
GEORGE CHAPPELL, QUE HUONG NGUYEN, Marshall University — We theoretically study the effect on the electronic structures and optical properties of a Co-doped semiconductor nanocrystal (NC) of the interaction between the impurity atom and an electron existing inside the NC. The optical properties of impurity centers in NCs are very different from the bulk cases. Beside the strong hybridization of *s*-*p*electrons of the semiconductor host and *d*electrons of the impurity due to confinement and the modification of the crystal field near the surface of the NCs, the Coulomb and exchange interaction of the d-electrons of the impurity centers with the confined electrons (or holes) existing inside the NCs could change the photoluminescence properties. In the strong confinement approximation, the boundary conditions enhance the coupling, and the effect on photoluminescence could be large. The transition $^4T_1 - ^2E$ of Co^{2+} has been considered. The exchange interaction between the extra electron and the states of the impurity ion together with the confinement effect mix the wave functions, split the impurity energy levels, break the previous selection rules, and change the transition probabilities. Energy, wave functions, luminescence efficiency, and transition lifetime have been calculated. The results imply that the PL intensity increases and the lifetime is shortened inside the NC.

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