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Optical Properties of Luminescent Centers in Bi-Doped Glass-Ceramics: A TD-DFT Study

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Theoretical modeling of electronic structures of heterostructure composites is a powerful tool for developing novel optical materials. This work presents the results of calculations of the excited electronic states and optical spectra of MoO_4 groups and Bi ions, considered potential luminescence centers in the glass-ceramic composite "$KBi(MoO_4)_2$ crystal@phosphate-molybdate glass of K_2O-P_2O_5-MoO_3-Bi_2O_3 system."
Atomic and electronic structures of the crystal, glass, and interphase layers were obtained using molecular dynamics and band-periodic density functional theory (DFT) methods. Geometry optimization was performed with the Gaussian software package. Excited electronic states were calculated using time-dependent DFT within a molecular cluster approach and the two-level ONIOM-2 method. The quantum mechanical (QM) region included the MoO_4 groups or Bi ions, while the mechanical (MM) region comprised all other atoms. Electronic embedding accounted for electrostatic interactions between QM and MM regions, treating QM atoms with TD-DFT and MM atoms as partial charges in the quantum-mechanical Hamiltonian.
Calculations were performed on ten structures of the glass and interphase regions, and results were averaged for statistical significance. Similar calculations were done for the MoO_4 groups and Bi ions in the $KBi(MoO_4)_2$ crystal. The results indicate significant differences in the optical absorption spectra of Bi atoms and MoO_4 groups across different regions of the composite.
Comparisons of the optical spectra for the crystal, glass, and interphase components with experimental data highlight the unique properties of each component. The origin of intrinsic luminescence in phosphate-molybdate glass-ceramics is discussed.

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