Photoluminescence in Ce-Doped Fluoride Borate Crystals

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Mechanisms of photoluminescence in antizeolite fluoride borates $LiBa_{12}(BO_3)_7F_4$ (LBBF)[1] doped by Ce^{3+} ions are interpreted based on a comparison between experimental and computational approaches. LBBF:Ce^{3+} demonstrates photoluminescence (PL) and holds promise for use as a phosphor in white light-emitting diodes. LBBFs are built of a porous framework $[Ba_{12}(BO_3)_6]^{6+}$ with channels along the *c* axis. Lattice channels can accommodate various guest anionic groups. In this study, we present the results of modeling the electronic and optical properties of Ce-containing fluoride borates where doping atoms are located at the different sites of the host lattice. Features on optical properties are caused by 5*d*-4*f* transitions on the Ce^{3+} ion. These states can serve as traps for electronic excitations and affect both the linear absorption and photoluminescent (PL) properties. PL spectra calculations were performed using two *ab initio* methodologies: (i) molecular dynamics (MD) sampling and (ii) time integration along with the progression of subsequently occupied excited states.[2] A combined experiment plus computation effort allows us to identify and interpret the most probable and most promising synthetic pathways to create the most efficient light emitter. The transition energy, intensity, and lifetime of cerium doped borate crystals depend on selection of a doping site. In addition to analysis of emission band contributed by cerium, this work did allow to identify and reproduce spectral lines hypothetically corresponding to the *intraband* transition in F-centers of borate crystals, in absence of metal center.

(1) Inerbaev, T. M.; Han, Y.; Bekker, T. B.; Kilin, D. S. Mechanisms of Photoluminescence in Copper-Containing Fluoride Borate Crystals. *J. Phys. Chem. C* **2022**, *126* (14), 6119-6128. DOI: 10.1021/acs.jpcc.1c10206.

(2) Vogel, D. J.; Kilin, D. S. First-Principles Treatment of Photoluminescence in Semiconductors. *J. Phys. Chem. C* **2015**, *119* (50), 27954-27964, Article. DOI: 10.1021/acs.jpcc.5b06434.