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Effect of fluorine on structure and luminescence properties of some oxide compounds

The electronic band structure for set of fluorine-doped oxide as well for oxyfluoride crystals were calculated by the Full-Potential Linear Augmented Plane Wave method. Calculations showed that fluorine impurities do not generate any states near band edges, consequently fluorine does not participate in optical transitions directly. Influence of fluorine on crystal structure is resulted in elongation of cation-anion bonds and can lead to increasing of luminescence intensity.

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