First principles calculations on the origin light photoluminescence emission in $CaTiO_3$, $BaWO_4$ and $SrTiO_3$

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The photoluminescence (PL) emission from CaTiO3 (CT), BaWO4 (BW)and SrTiO3 (ST) crystalline, quasi-crystalline, and quasi-amorphous samples, prepared by the polymeric precursor method, was examined by ab initio quantum mechanical calculations. It was used in the modeling the structural model consisting of one pyramidal TiO5 or WO3 unit piled upon the TiO6 or WO4, which are representative of disordered structures of quasi-crystalline structures such as ST, BW and CT. The structural crystallization process was monitored by X-ray diffraction. In quasi-crystalline powders, the photoluminescence (PL) in the visible region showed different peak positions and intensities in CT, BW and ST. The PL emission was linked to distinct distortions in lattices and the emission in CT, BW and ST—was also examined in the light of favorable structural and electronic conditions.
Keywords: Ab initio calculations, photoluminescence

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