Abstract Submitted
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Ab initio study of Cu doped KCl[1] ROBERTO NUNEZ-GONZALEZ, Universidad de Sonora. Departamento de Matematicas, RAUL ACEVES-TORRES, ALVARO POSADA-AMARILLAS, Universidad de Sonora. Departamento de Investigacion en Fisica — Experimental studies have shown that doping alkali halides with copper atoms result in an enhancement of their optical properties. In this work, we calculate the electronic properties of KCl doped with Cu through the Density Functional Theory (DFT) scheme. The Wien2k was used, which is based on the Full-Potential Augmented Plane Waves with local orbital method (APW-lo). Structural optimization of the 3x3x3 supercell was performed using the GGA PBE96 approximation to exchange-correlation. For band gap and electronic properties, calculations were performed using the modified Becke-Johnson potential (mBJ). Band structure, density of states and optical properties are examined and compared with the properties of pure KCl.

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