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Electronic properties of doped cesium niobate LU WANG, RENAT SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, ROBERT SMITH, Department of Chemistry, University of Nebraska at Omaha, Omaha, NE 68132, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588 — Antiferroelectric cesium niobate $Cs_2Nb_4O_{11}$ (CNO) is known to have novel water splitting capability. It was reported that the broad blue photoluminescence was observed at 77 K. Particularly when treated with NiO_2, the water-splitting activity under UV-light irradiation increased five times. In this work we present systematic studies of the electronic properties of doped CNO by using density functional theory calculations. We first obtain direct band gap of 3.12 eV for the pure sample that agrees well with experimental value of 3.55 $\pm$ 0.05 eV. Then we notice, at both the high and low-density regions, the band gap effectively reduced after oxygen atoms substituted by sulfur and nitrogen, and niobium by vanadium. As a final point, we present and discuss relations between impurity concentration and band gap reduction.

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