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ELECTRONIC AND OPTICAL PROPERTIES UNDER PRESSURE EFFECT OF ALKALINE EARTH OXIDES MgO, CaO AND SrO

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ABSTRACT: We report results of first-principles calculations for the electronic and optical properties under pressure effect of MgO, SrO and CaO compounds in the cubic structure, using a full relativistic version of the full-potential augmented plane-wave (FP-LAPW) method based on density functional theory, within the local density approximation (LDA) and the generalized gradient approximation (GGA). Moreover, the alternative form of GGA proposed by Engel and Vosko (GGA-EV) is also used for band structure calculations. The calculated equilibrium lattices and bulk modulus are in good agreement with the available data. Band structure, density of states, and pressure coefficients of the fundamental energy gap are given. The critical point structure of the frequency dependent complex dielectric function is also calculated and analyzed to identify the optical transitions. The pressure dependence of the static optical dielectric constant is also investigated.

KEYWORDS: FP-LAPW; alkaline earth oxides; band-gap pressure coefficient