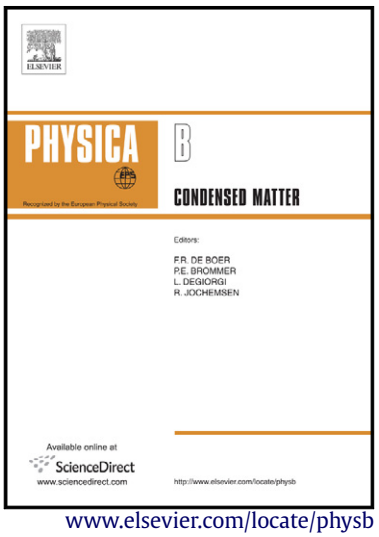


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# Electronic structure of lanthanum sesquioxide: A Compton scattering study

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**ABSTRACT**

We present the first-ever experimental and theoretical momentum densities of $La_2O_3$. The Compton line shape is measured using a 20 Ci $^{137}Cs$ Compton spectrometer at an intermediate resolution with full width at half maximum of 0.34 a.u. The experimental Compton profile is compared with the theoretical electron momentum densities computed using linear combination of atomic orbitals (LCAO) method with density functional theory (DFT). It is seen that the generalized gradient approximation (GGA) within DFT reconciles better with the experiment than other DFT based approximations, validating the GGA approximation for rare-earth sesquioxides. The energy bands and density of states computed using LCAO calculations show its wide band gap nature which is in tune with the available reflectivity and photo-absorption data. In addition, Mulliken's population and charge density are also computed and discussed.

**Keywords:** Compton scattering, Electronic structure, Density functional theory

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