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The nature and origin of electronic gap in perovskite and post-perovskite $CaIrO_3$ VIJETA SINGH, JIJI PULIKKOTIL, CSIR- National Physical Laboratory — Accumulated experimental data and theoretical studies derive little consensus on the insulating ground state of $CaIrO_3$. While in post-perovskite $CaIrO_3$, the origin of the electronic gap is associated with Coulomb correlations, Spin-orbit coupling, long range antiferromagnetic ordering of the Ir ions and/or as a cooperative effect, perovskite $CaIrO_3$ is found to be a semi-metal. Using comprehensive calculations, based on density functional theory, we find that post-perovskite $CaIrO_3$ is a slater-type antiferromagnetic insulator, while its orthorhombic perovskite counterpart is a semi-metal. We owe the discrepancies in the theoretical calculations, to the choice of the exchange correlation potential. Our mBJ calculations correctly reproduce the experimental observed properties of pPv- $CaIrO_3$, such as the magnitude of the Ir moment and electronic gap, large crystalline anisotropy etc. On the other hand, the transport properties calculated using BTE in CSTA for pv- $CaIrO_3$ clearly shows the semi-metallic characteristics of the system.

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