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Study of the ionic conductivity in $Ce_{1/3}NbO_3$ JOSE FRANCISCO GOMEZ GARCIA, GUSTAVO TAVIZON, Fac. de Quimica, PABLO DE LA MORA, Fac. de Ciencias, Universidad Nacional Autonoma de Mexico — $Ce_{1/3}NbO_3$was synthesized using stoichiometric quantities of CeO_2 and Nb_2O_5 and heated for 48h at 1350^oC in air. The electric conductivity was measured in the 25^oC-1000^oC interval. A small gap of 0.25-0.78eV was found. To study the origin of the transport DFT calculations were carried out; the results show a 0.4eV gap, but since the gaps are not correctly predicted with DFT, a further calculation with a modified Becke-Johnson (mBJ) potential was carried out obtaining a gap of 2eV, but a Ce 4f peak was found at the Fermi energy (E_F). When an intra-atomic repulsion term was added (LDA+U) the Ce 4f peak moved down and a 2.4eV gap was found. The calculations show that the conductivity does not have electronic origin but ionic. Atomistic calculations rule out that the transport is due to the Ce ions; on the other hand, these calculations agree very well with oxygen ions as charge carriers in this material.

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