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Calculation of the gap in $Ce_{1/3}NbO_3$ PABLO DE LA MORA, Facultad de Ciencias, JOSE FRANCISCO GOMEZ GARCIA, Facultad de Quimica, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico
— With experimental measurements, $Ce_{1/3}\ NbO_3$ was found to have a small gap of *0.25-0.78eV*. In order to find whether this gap is due to electronic origin *ab-initio DFT* (*WIEN2k*) calculations were done. To find the correct gap, the calculations were done using a modified Becke-Johnson (*mBJ*) potential. A 'conducting' *Nb-O* gap with a *Ce:4f* peak in the middle was found. In the convergence process, due to the nature of the *mBJ* potential, this *Ce:4f* interfered with the Fermi energy E_F. To avoid this problem a Hubbard U_H was added to the *Ce* atom, then it was possible to extrapolate back and obtain the correct 'conducting' *Nb-O* gap of *2eV* with the *Ce:4f* peak at *1.3eV* from the lower end of the gap. With this it can be confirmed that the conduction is not of electronic nature.

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