First principles study of native defects in BeO

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Using first principles calculations within the formalism of the Density Functional Theory (DFT) and the Local Spin Density Approximation (LSDA) for the exchange-correlation term, we studied native defects (vacancies and antisites) in wurtzite Beryllium Oxide (BeO). The ion-electron interactions are modulated by Ultrasoft Vanderbilt Pseudopotentials and the Khon-Sham (KS) orbitals are described by a Plane Wave (PW) basis set with an energy cutoff of 400 eV. To avoid the non realistic effect due a "periodic" doping we use the supercell approximation. Our results show that the wurtzite (w-BeO) is the most stable structure and the calculated bandgap for the w-BeO is 7.9 eV. The stability of the defects (X is an anti site or vacancy) are analyzed by calculated the formation energies (\(E_{\text{form}}\)) through total energy calculations (\(E_t\)), according to the equation

\[
E_{\text{form}}(X) = E_t[X] - n_O\mu_O - n_{Be}\mu_{Be}.
\]

In this equation, \(n_O\) (\(n_{Be}\)) and \(\mu_O\) (\(\mu_{Be}\)) represent the number and the chemical potential of the Oxygen (Beryllium) atoms in the X defect, respectively. The chemical potentials for Oxygen and Beryllium are calculated as the total energy per atom of the most stable configuration. In this work we use the \(O_2\) molecule and the Be bulk structure to calculate the oxygen and Beryllium chemical potentials, respectively. The atomic chemical potential are constrained by the thermodynamic equilibrium condition:

\[
\mu_O + \mu_{Be} = \mu_{BeO}^{\text{bulk}}.
\]

Where, \(\mu_{BeO}^{\text{bulk}}\) is the total energy for a BeO pair in the hexagonal (wurtzite) BeO structure. Two extreme conditions can be established: The Be-rich (O-rich) case should be attained when the system is assumed to be in equilibrium with the Be bulk (\(O_2\) molecule). In this case, \(\mu_{Be} = \mu_{Be}^{\text{bulk}}\) (\(\mu_O = \mu_{O\text{molec}}\)) and the oxygen (beryllium) chemical potential, is given by the thermodynamic equilibrium condition.

Between all the defects studied, the oxygen vacancy (\(V_O\)) is the most stable defect (lowest formation energy), while the Beryllium in the Oxygen site (\(Be_O\)) is the less stable defect. For the vacancies we obtained formation energies of the 0.75 eV (7.88) and 9.16 eV (2.02) for the \(V_O\) and \(V_{Be}\) in a Be-rich (O-rich) growth condition. For the antisites we obtained formation energies of the 16.08 eV (1.76) and 6.69 eV (20.95) for the \(O_{Be}\) and \(Be_O\) in the Be-rich (O-rich) growth conditions.

Furthermore, we observe that those defects introduce deep and localized electronic levels in the band gap. Those defects must rule the origin of the luminescent properties of BeO[1]. For the \(V_{Be}\) a local spin magnetic moment of 2 \(\mu_B\) (\(\mu_B\) is the Bohr magneton) is obtained.