Structural, Electronic, and Thermodynamic Properties of the T and B Phases of Niobia: First-Principle Calculations

Pinto, Mirele B.

Soares, Antonio Lenito

Mella Orellana, Andy

Duarte, Hélio A.

De Abreu, Heitor A.

 Different polymorphs of Nb2O5 can be obtained depending on the pressure and temperature of calcination leading to different catalytic properties. Two polymorphs of niobia, T-Nb2O5 and B-Nb2O5, have been investigated by means of density functional/plane waves method. The equation of state predicted that B-Nb2O5 phase is more stable than the T-Nb2O5 at low temperature; however at high pressure both phases are stable. These results are in good agreement with the available experimental data. The calculated cohesive energies of 6.63 and 6.59 eV·atom-1 for the B-Nb2O5 and T-Nb2O5, respectively, also corroborate this conclusion, and it can be compared to the experimental value of 9.56 eV atom-1 estimated for the most thermodynamically stable phase. The topological analyses based on quantum theory of atoms in molecules (QTAIM) and electron localization function (ELF) were applied and reveal bonds with large ionic character for both phases. The B-Nb2O5 presente