Czestochowa University of Technology

Faculty of Production Engineering and Materials Technology

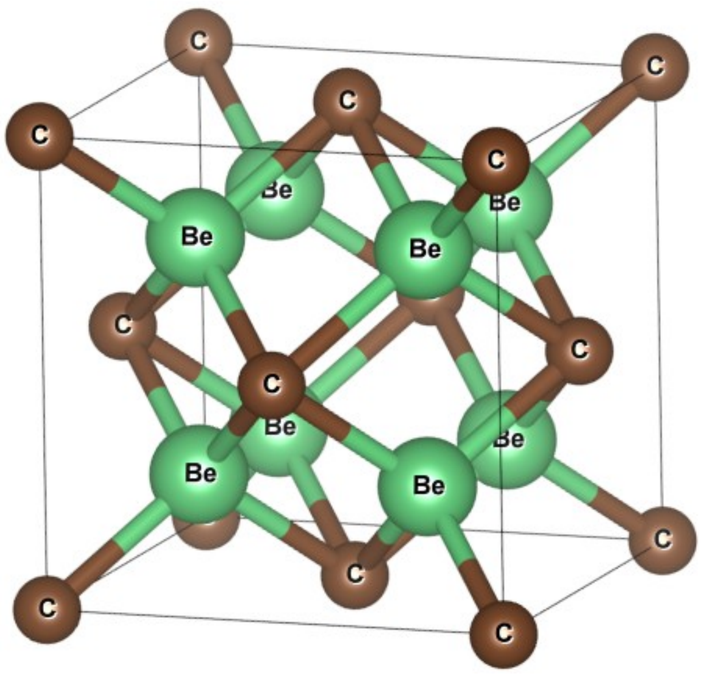
Ave. Armii Krajowej 19, 42-200 Czestochowa, Poland

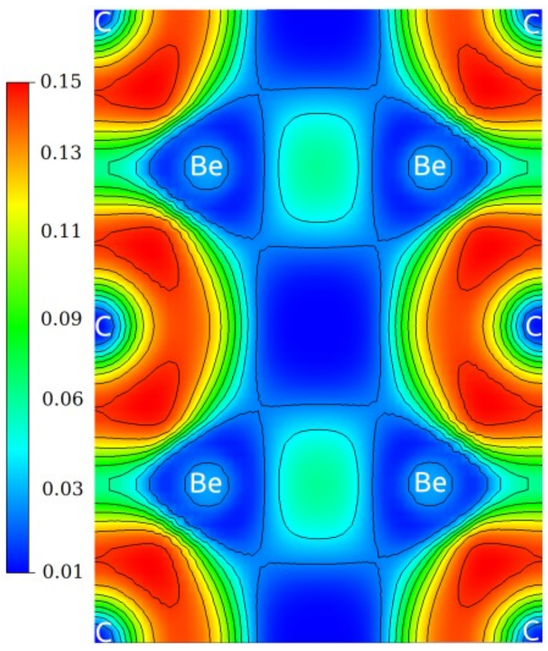
A first principle study of structural and electronic properties of CBe_2 compound.

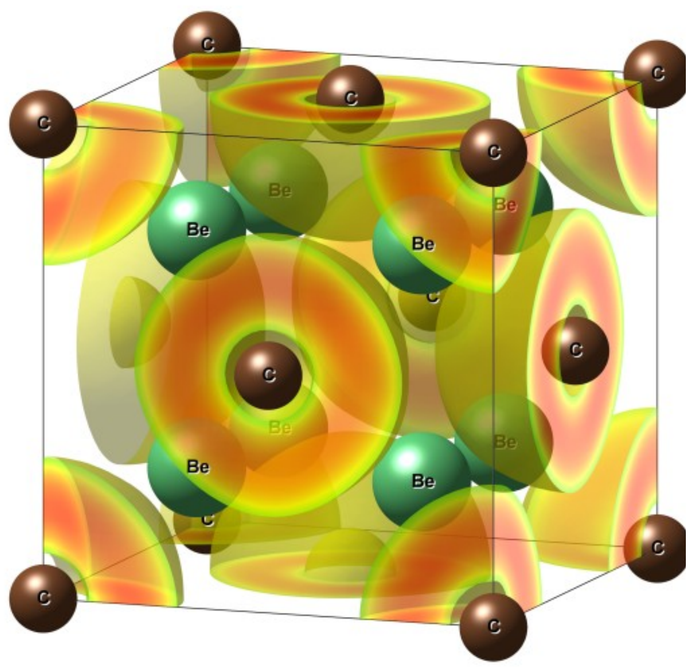
Konrad M. Gruszka

Czestochowa University of Technology, 42-201 Czestochowa, Poland

In this paper a DFT-based study of the structural and electronic properties at ambient pressure of pure beryllium carbide (CBe_2) phase are presented. The PBE-GGA approach as implemented in the Quantum Espresso electronic structure code was used through scalar-relativistic calculation. A structural equilibrium parameters and bulk modulus were also calculated. Obtained results show that phase is semiconducting in nature with a band gap equal to 1.22 eV. Electronic properties in terms of band structure and density of states are presented. Calculations show that magnetic ordering is not favorable and total magnetic moment is zero. Using electron localization function and Bader charge analysis we determined bonding character inside Be_2C.

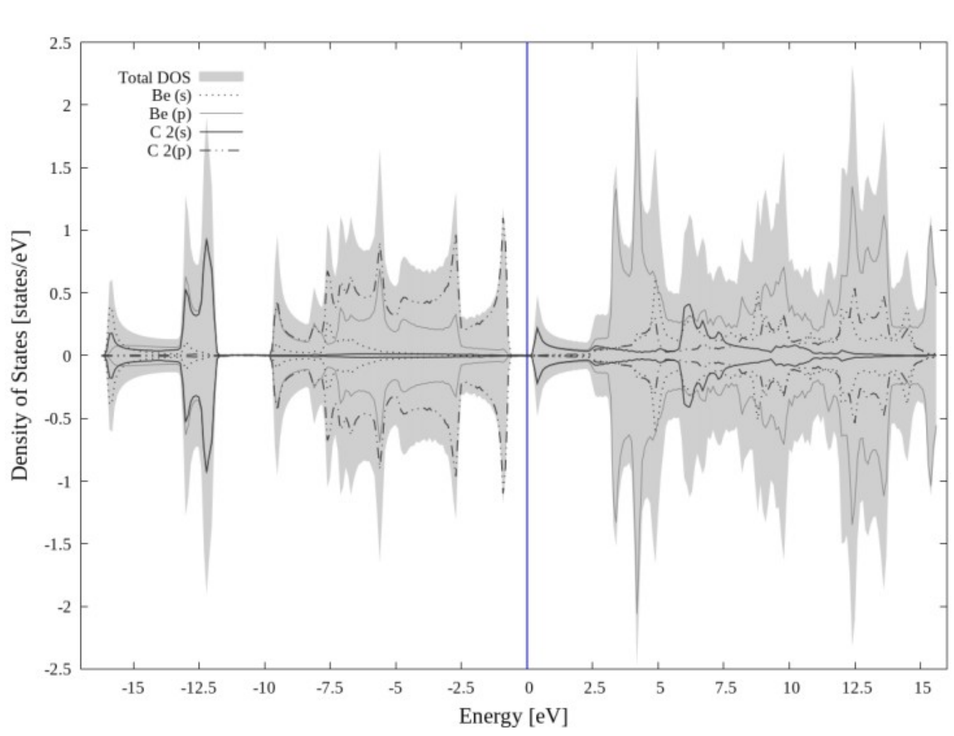






The calculated bulk modulus of 180 GPa means that material is rather hard to compress. From the conducted electronic analysis the semiconducting nature of compound is revealed with indirect band gap of 1.22 eV. The frontier molecular orbital as shown in PDOS figure consists mainly of C-2(p) shell which in connection with Be 2(p) shell is mainly responsible for stabilization due to strong mixing below Fermi level. By utilizing electron localization function the nature of bonding was specified. The bonding between carbon and beryllium is of ionic nature, while bonding between nearest Be has covalent character. The Bader charge analysis seems to confirm this observation, showing additional charge accumulated at carbon ions wile charge is depleted from beryllium.

Projected density of states of CBe_2. The blue vertical line denotes Fermi level



Band structure and DOS of CBe_2