

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study of two-dimensional electride: Yttrium carbide CHANDANI NANDADASA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, Starkville, MS 39762, USA, YOUNG LEE, SUNG KIM, Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Department of Energy Science, Sungkyunkwan University, Korea — Electrides are an exclusive class of ionic compounds in which electrons serve as anions. We have performed first-principles density functional theory (DFT) calculations to investigate the structural, electronic and magnetic properties of two-dimensional layered-structure yttrium carbide (Y_2C). Generalized gradient approximation (GGA) with Projector Augmented Potentials (PAW) was used to obtain optimized lattice parameters, energy band structure, charge density and density of states (DOS) plots for Y_2C . The theoretically predicted structure of Y_2C is in good agreement with the experimental results. The band crossing the Fermi energy level proved that Y_2C has metallic properties. Additionally projected electronic density of states profiles were obtained to identify the electronic contribution from Y, C and non-atomic orbital located in interstitial site. The results of these calculations indicate that the presence of trapped electrons within the Y_2C interlayers. Furthermore, surface energies of Y-Y and Y-C were calculated and charge densities were plotted with these surfaces. Magnetization density plots were used to obtain magnetic properties.

Chandani Nandadasa
Mississippi State University

Date submitted: 14 Nov 2014

Electronic form version 1.4