MODELING OF ELECTRONIC AND OPTICAL PROPERTIES OF C_3N_4 WITHIN DFT FRAME

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Abstract. The electronic and optical properties of bulk-, supercell- and nanocluster-C_3N_4 are studied by the first-principles calculations within the framework of the density functional theory (DFT). From the density of states of carbonitride, it was found that valence band occupied by N 2p states, conduction band occupied by C 2p states. The light permeability spectrum displays the wide photoconductive response interval and a high peak of C_3N_4.

DFT [1] is the most propagated approach in first principles calculations of realistic systems. This method plays an important role in condensed matter theory and material sciences. The electronic structure determines the basic properties of matter such as electric, magnetic, thermal and mechanical.

In adiabatic approximation we exclude dense small size nuclei from consideration and reduce multi-atomic system to multi-electron system. In order to discuss these systems, we make further reduction of multi-electron problem to single-electron by considering of the motion of electron in the field of others. For this approach Hartree–Fock method [2] was developed. The main disadvantage of approximation is ignoring of the spin correlation energy between antiparallel electrons, while DFT considering the correlation energy of electrons within exchange-correlation therm. DFT established on Hohenberg-Kohn Theorem [3], its core idea is to use the density of particles to reflect properties of the ground states of molecules, atoms and solids, so that the corresponding electronic structure and total energy can be obtained. However, Hohenberg-Kohn theorem cannot solve because of the difficulty of the interaction term in kinetic energy functional, so Kohn-Sham equation [4] is proposed.

The calculations of C_3N_4 were performed within DFT frame by using plane-wave pseudopotential approach in CASTEP codes [5]. Modeling of bulk C_3N_4 and supercell 2×2×2, we used generalized gradient approximation of PBE to describe exchange-correlation potential. Energy cutoff of plane-wave was set to be 450 eV, the special points sampling integration over the Brillouin zone were performed using a k-mesh of dimensions 2×2×2 k-points mesh according to a Monkhorst–Pack scheme.

The result show that C_3N_4 is an indirect gap semiconductor, the bandgap value of bulk and supercell is 3.812eV, 3.806eV, in the case of a nanocluster, the formation of broken bonds on the surface occurs, which is manifested in the formation of a peak at the Fermi level, the valence band occupied by N 2p states, the conduction band occupied by C 2p states. The optical properties of C_3N_4 (Fig. 1) show there are two absorption peaks for light absorption in the ultraviolet region, in the case of a nanocluster, a second peak is blurred due to the appearance of surface states. The light permeability spectrum displays wide photoconductive response interval and a high peak of C_3N_4.

These results demonstrate that the materials C_3N_4 with good optical conductivity is prospective in the field of photoelectric equipment.

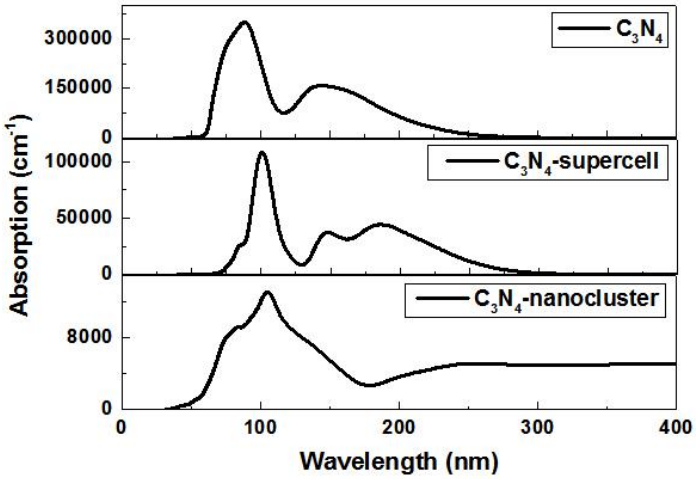

Fig. 1. The absorption of C_3N_4.

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