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Electronic structure, charge density, and chemical bonding properties of $C_{11}H_8N_2O$ o-methoxydicyanovinylbenzene (DIVA) single crystal

Abstract

A comprehensive theoretical density functional theory (DFT) study of the electronic crystal structure, bonding properties, electron charge density of $C_{11}H_8N_2O$ o-methoxydicyanovinylbenzene (DIVA) single crystals were performed. The exchange and correlation potential was described within a framework of the local density approximation (LDA) by Ceperley-Alder and gradient approximation (GGA) based on exchange-correlation energy optimization to calculate the total energy. In addition, we have used Engel-Vosko generalized gradient approximation (EV-GGA) and the modified Becke-Johnson potential (mBJ) for the electronic crystal structure, bonding properties, electron charge densitycalculations. There is systematically increasing in the energy gap from 2.25 eV (LDA), 2.34 eV (GGA), 2.50 eV (EV-GGA), 2.96 eV (mBJ). Our calculations show that this crystalpossess direct energy gap. Furthermore, the electronic charge density space distribution contours in the (1 1 0) crystallographic plane clarifies the nature of chemical bonding.

Keywords — Theoretical density, electronic charge density, crystallographic plane, generalized gradient approximations.