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ELECTRONIC AND STRUCTURAL PROPERTIES OF Sr_2VO_3FeAs

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Abstract

The band structure, total density of states (DOS) and electronic density and bound length in ground state of new superconductor Sr_2VO_3FeAs are calculated by the using full potential-linearized augmented plane wave (FP-LAPW) method in the framework of density functional theory (DFT) with the generalized gradient approximation (GGA) by WIEN2k package. From the DOS analysis, as well as charge-density studies, we have concluded that the bonding between Sr-Sr and Sr-O is ionic and bonding between Fe-As is covalent.

Keywords and phrases: band structure, Sr_2VO_3FeAs, WIEN2k, FP-LAPW, DFT, GGA.

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