Electronic properties of chrome-doped Zinc sulphide nanosheet

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Abstract

Zinc sulphide (ZnS) is a semiconductor with a wide band gap of about 3.77 eV. Based on the recent achievements regarding the electronic applications of this material, in the present work, we are going to investigate the electronic properties of the pure and Cr-doped ZnS nanosheet within the framework of density-functional theory (DFT) implemented in Quantum Espresso package using the General Gradient Approximation (GGA) with a Pedrew-Burke-Ernzerhof (PBE) describing the correlation potential. Results verify that doping the Cr atoms reduces the band gap down to 1.5 eV, yielding half-metallic properties for the ZnS nanosheet.

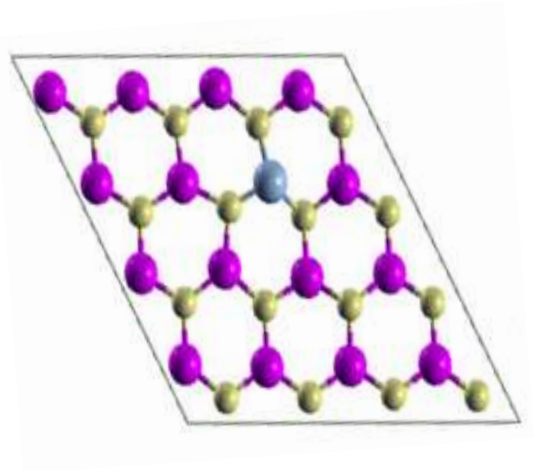

Figure 1. Cr-ZnS nanosheet