Density functional theory study of bulk and single-layer magnetic semiconductor $CrPS_4$

Houlong L. Zhuang[1,*] and Jia Zhou[2]

[1]Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA
[2]MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 1500001, China
*Current address: School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona 85287, USA.

Searching for two-dimensional (2D) materials with multifunctionality is one of the main goals of current research in 2D materials. Magnetism and semiconducting are certainly two desirable functional properties for a single 2D material. In line with this goal, here we report a density functional theory (DFT) study of bulk and single-layer magnetic semiconductor $CrPS_4$. We find that the ground-state magnetic structure of bulk $CrPS_4$ exhibits the A-type antiferromagnetic ordering, which transforms to ferromagnetic (FM) ordering in single-layer $CrPS_4$. The calculated formation energy and phonon spectrum confirm the stability of single-layer $CrPS_4$. The band gaps of FM single-layer $CrPS_4$ calculated with a hybrid density functional are within the visible-light range. We also study the effects of FM ordering on the optical absorption spectra and band alignments for water splitting, indicating that single-layer $CrPS_4$ could be a potential photocatalyst. Our work opens up ample opportunities of energy-related applications of single-layer $CrPS_4$.