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Ab initio study of magnetic single layer MPX3 metal-phosphorous-trichalcogenides BHEEMA LINGAM CHITTARI, EUYHEON HWANG, Sungkyunkwan University, JEIL JUNG, University of Seoul, ALLAN H. MACDONALD, The University of Texas at Austin — We analyze the electronic structure of two dimensional (2D) MPX3 (M= V, Cr, Mn, Fe, Co, Ni, Cu, Zn, and X = S, Se, Te) transition metal thiophosphates, viewing them as single layer van der Waals materials that can exhibit magnetic order. Our ab initio calculations for MPX3 single layer compounds predict both semiconducting phases with variable band gap sizes and metallic phases, and an intimate interplay between magnetic order and the presence of a gap. A systematic trend of decreasing band gaps in antiferromagnetic states is observed as the chalcogen atoms S, Se, and Te change from smaller to larger atomic number, Ferromagnetic, antiferromagnetic, and non-magnetic phases, and lattice constant changes accompanied by distortions in crystal symmetry, occur as the metal atom is varied. The sensitive interdependence between magnetic, structural, and electronic properties suggests the important potential of this class of 2D magnetic van der Waals materials for strain and field-effect carrier tunable spintronics.

Bheema Lingam Chittari
Sungkyunkwan University

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