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Effects of the Hubbard U correction on the electronic and magnetic properties of tetragonal V_2P_2 sheet

Yusuf Zuntu Abdullahi[a1], Sohail Ahmad[b] Abdullahi Abdu Ibrahim[c]

[a]*Department of Physics, Faculty of Science, Kaduna State University, P.M.B. 2339 Kaduna State, Nigeria.*

[b]*Department of Physics, College of Science, P O Box 9004, King Khalid University, Abha, Saudi Arabia.*

[c]*Computer Engineering Department, Altinbas University, Istanbul, Turkey*.

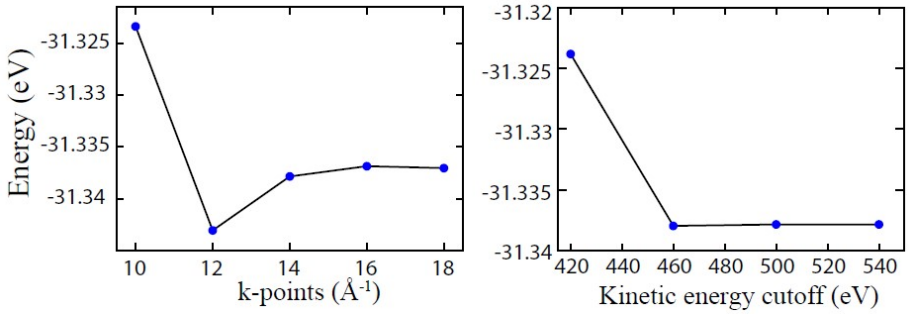

Fig. S1 Total energy of V_2P_2 sheet as function of Monkhorst-pack (**Left**) and wave function cutoffs (**Right**).

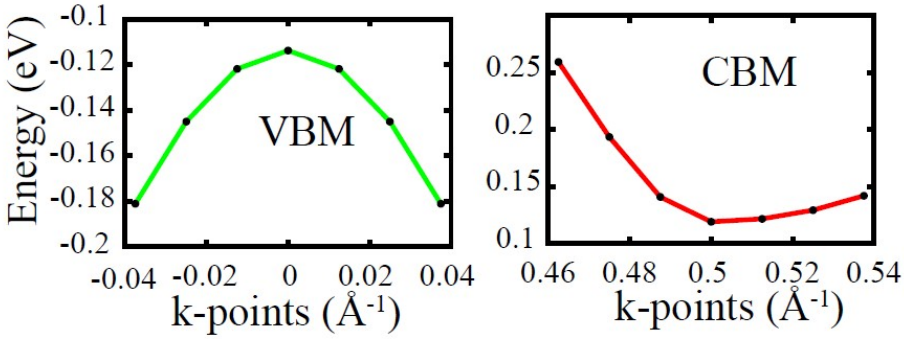

Fig. S2 The E-k points closed to the CBM and VBM plots for V_2P_2 sheet.

[1]Corresponding author.
Email address: *yusufzuntu@gmail.com*

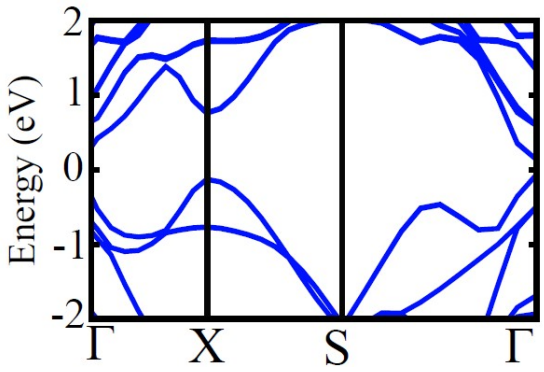

Fig. S3. The electronic band structure using the HSE functional for t-V_2P_2 sheet.

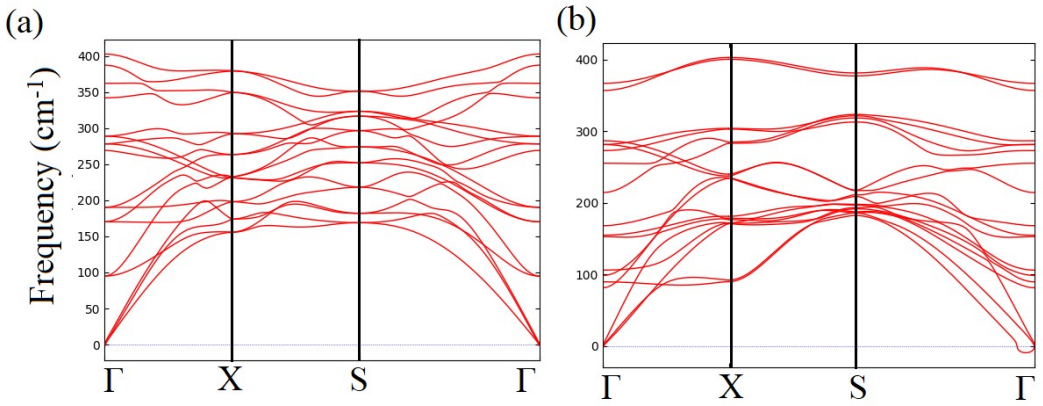

Fig. S4. The phonon dispersions curves obtained using the (a) PBE and (b) PBE+U for t-V_2P_2 sheet

Table S1 The atomic positions and lattice constant for the tetragonal V_2P_2 sheet.

System	L (Å)	Atomic positions			
PBE	$a = b =$ 3.160 Å	V	-0.004719727	1.576723644	12.119697907
		V	1.576723022	-0.004719159	13.727120004
		P	-0.004134114	1.576138120	14.611705249
		P	1.576138501	-0.004134923	11.235097521
PBE+U	$a = b =$ 3.360 Å	V	0.012684338	1.692784585	6.511549618
		V	1.692784599	0.012685324	8.488466319
		P	0.012602591	1.692851786	9.193939943
		P	1.692850606	0.012603159	5.806043166

Table S2 The atomic positions and lattice constant for the orthorhombic V_2P_2 sheet.

System	L (Å)	Atomic positions			
PBE	$a =$ 3.886 Å $b =$ 2.815 Å	V	1.942844987	0.000129200	7.986247063
		V	3.885580301	2.815611839	9.484710693

		P	0.000040889	1.407861710	7.409172058
		P	1.942767501	1.407879472	10.061764717

Table S3: Relative energies (eV) between orthorhombic (E_O) and tetragonal (E_T) V_2P_2 sheet.

Sheet	$E_T - E_T$	$E_O - E_T$
V_2P_2	0	0.911

Table S4: The calculated carrier effective mass (m^*) for tetragonal V_2P_2 sheet.

Sheet	Carrier	m^*/m_0
V_2P_2	h	3.162
	e	2.656

Table S5. Geometry and electronic structure for V_2P_2 with adsorbed Li, Na, K, Ge, and Si atoms. The favorable adsorption site (Ads. Site) for Li, Na, K, Ge, and Si atoms on the T_V, T_V, T_V, T_H and T_H sites respectively. T_V and T_H represent top of the V atom and hollow sites on (2x2) supercell of the V_2P_2 sheet. X refers to an adsorbate species. E_{ads}, $d_{V_2P_2-X}$ refer to adsorption energy and averaged bond length between V_2P_2 sheet and the adsorbates. M_{cell} stands for magnetic moment per unit cell. EC refers to the electronic character of the V_2P_2 with adsorbates. In the present systems, the EC is found to be metallic (M).

System	Ads. Site	E_{ads} (eV)	$d_{V_2P_2-X}$ (Å)	M_{cell} (μ_B)	EC
Li	T_V	2.40	2.51	0.50	Metal
Na	T_V	1.87	2.84	1.00	-
K	T_V	1.94	3.23	1.00	-
Ge	T_H	3.53	2.35	0.00	-
Si	T_H	4.02	2.24	0.00	-