Supporting Information

Versatile Electronic and Magnetic Properties of Corrugated V_2O_5 Two-Dimensional Crystal and Its Derived One-Dimensional Nanoribbons: A Computational Exploration

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Table 1 The plane-wave cut off energy testing results based on bulk V_2O_5, the k-point mesh is chosen as 4×8×8.

Cut off (eV)	Spin-nonpolarized energy (eV)	Spin polarized energy (eV)	Magnetization (μ_B)
360	-117.194	-117.195	0.0027
400	-116.976	-116.979	0.0022
450	-116.816	-116.817	0.0012
500	-116.814	-116.815	0.0009
550	-116.712	-116.712	0.0007
600	-116.801	-116.800	0.0006
700	-116.863	-116.864	0.0006

From Table 1, we see that the spin polarized magnetic moment becomes converged when the cut off is larger than 600 eV, and the energy difference between 600 eV and higher cut-off is less than 0.1 eV, so we choose the cut-off (600 eV) as our computation parameter.

To test the effectiveness of this method, we presented the optimized structure of bulk V_2O_5 based on PBE and PBE-D2 approaches, respectively (shown in Figure S1). The PBE yields a nearest interlayer V-O distance between adjacent layers of 3.31 Å, whereas PBE-D2 predicts a corresponding V-O distance of 2.85 Å, which is more comparable with the experimental value of 2.79 Å.[i] The intralayer V-O bond lengths within a corrugated plane obtained using PBE and PBE-D2 are similar. Thus PBE-D2 is quantitatively better than PBE when dealing with the weak-bonded layer system.

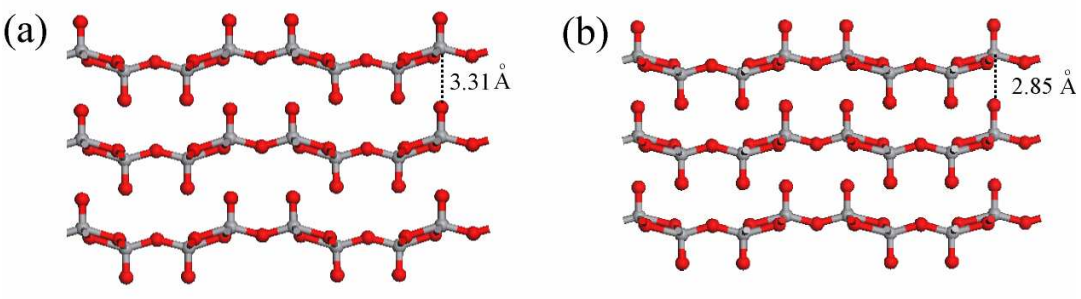

Figure S1. The optimized geometry of bulk V_2O_5 based on PBE (a) and PBE-D2 (b), the labeled bond length is the nearest V-O distance between two adjacent layers.

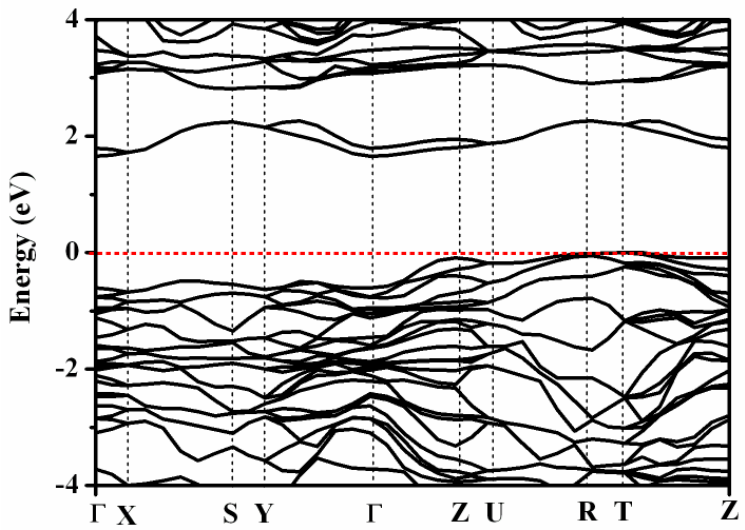

Figure S2. Band structure of bulk V_2O_5. The bands are plotted along a path connecting high-symmetry points in the irreducible Brillouin zone. The Fermi energy is denoted by a red dashed line.

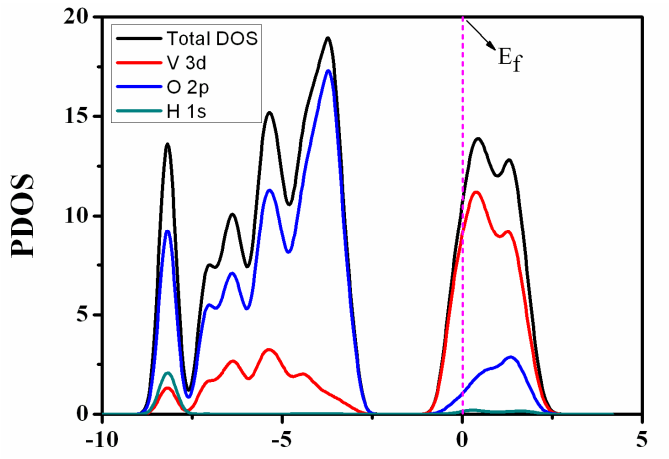

Figure S3. Partial density of states (PDOS) of surface-hydrogenated single layer V_2O_5 projected into different atom orbitals.

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[i] Enjalbert, R.; Galy, J. A Refinement of the Structure of V_2O_5. *Acta cryst. C* **1986**, *42*, 1467-1469.