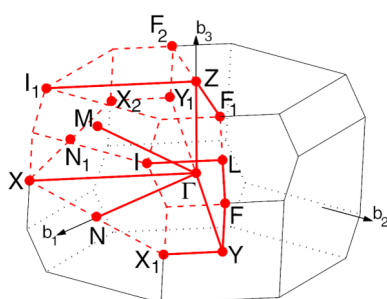


Doping isolated one-dimensional antiferromagnetic semiconductor Vanadium tetrasulfide (VS_4) nanowires with carriers induces half-metallicity

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1 Figures



MCLC₁ path: Γ -Y-F-L-||I₁-Z- Γ -X|X₁-Y|M- Γ -N|Z-F₁

Figure S1: The high symmetry points of the first Brillouin zone for the band structure of the VS_4 bulk phase. This figure was created from <http://materials.duke.edu/awrapper.html>

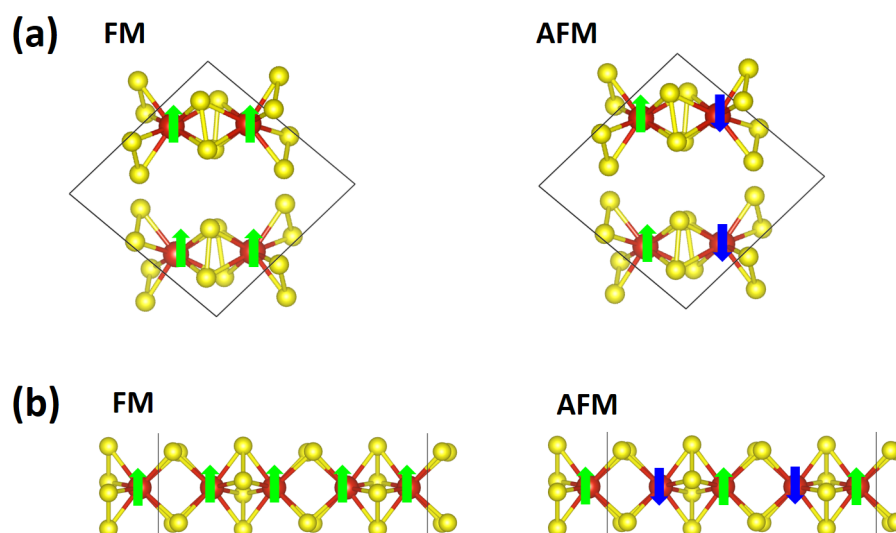


Figure S2: Ferromagnetic (FM) and antiferromagnetic (AFM) states for (a) VS_4 bulk phases and (b) isolated VS_4 nanowires (NWs).

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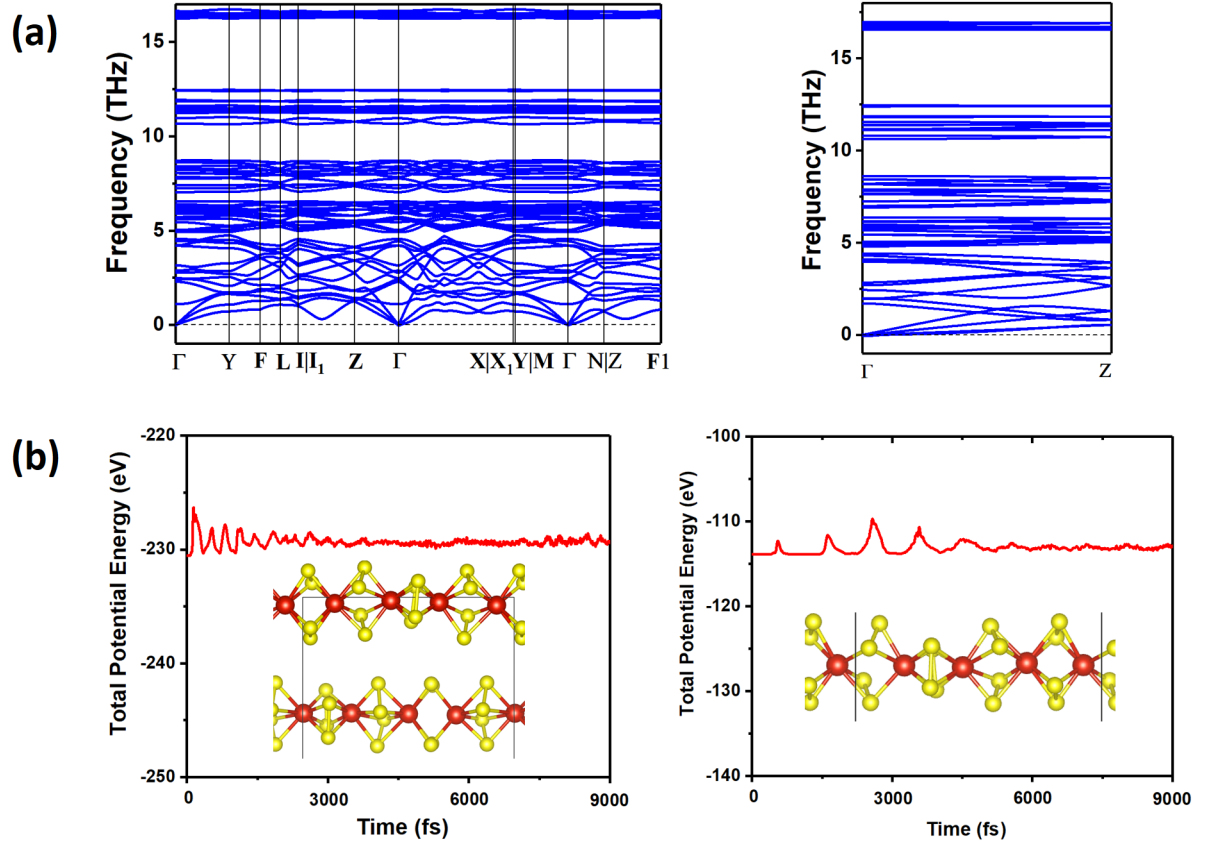


Figure S3: (a) Phonon spectra and (b) total potential energy of NWs as a function of simulation time for the VS₄ bulk phase (conventional cell) and the isolated VS₄ NW by using *ab-initio* molecular dynamics (300K). The inset shows the corresponding structure after the simulation for 9 ps.

T_N is defined as a maximum on the temperature dependent specific heat C_V curve,

$$C_V = (\langle E^2 \rangle - \langle E \rangle^2)/T^2 \quad (1)$$

Where T is the temperature and E is the energy.

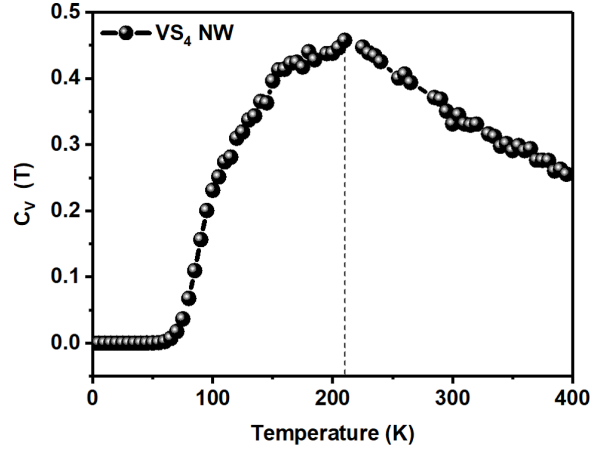


Figure S4: Specific heat calculated for the isolated VS_4 NW with respect to the temperature

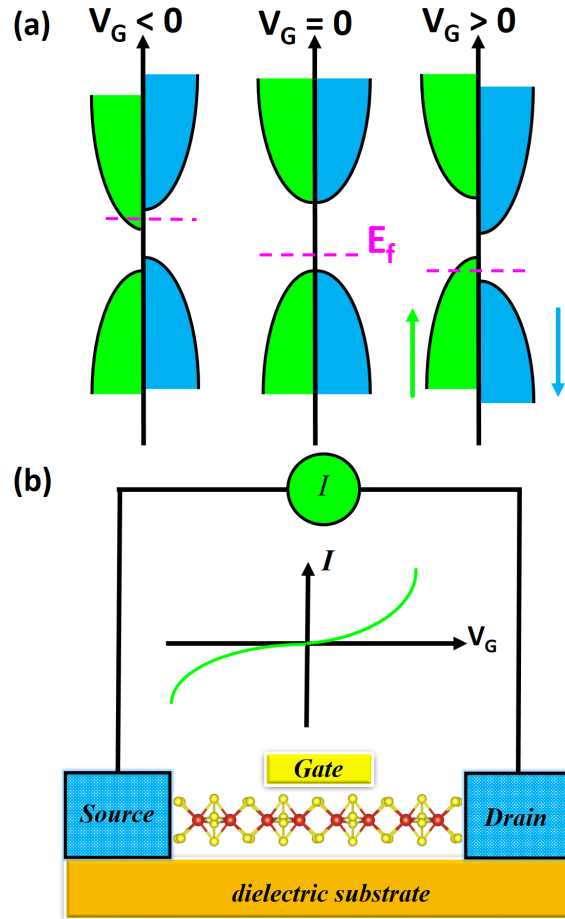


Figure S5: (a) The schematic plot of transformation between the HMAF and AFM states under gate voltages of $V_G < 0$, $V_G = 0$ and $V_G > 0$, respectively. (b) The schematic plot of AFM spintronics device based on the isolated VS_4 NW, together with the $I - V_G$ relationship under the gate voltage. The switching of the spin current can be manipulated by gate voltages.

To evaluate the stability of the isolated VS_4 NW inside BN nanotubes of different sizes, the binding energy (E_b) for the unit cell is calculated as:

$$E_b = E_{\text{total}} - E_{\text{NW}} - E_{\text{nanotube}} \quad (2)$$

where E_{total} stand for the total energies of the isolated VS_4 NW inside the (m, m) BN nanotube. E_{NW} and E_{nanotube} are the energies of the isolated VS_4 NW and the (m, m) BN nanotube. $m = 6, 7, 8$ and 9 , which are the direction of the vector.

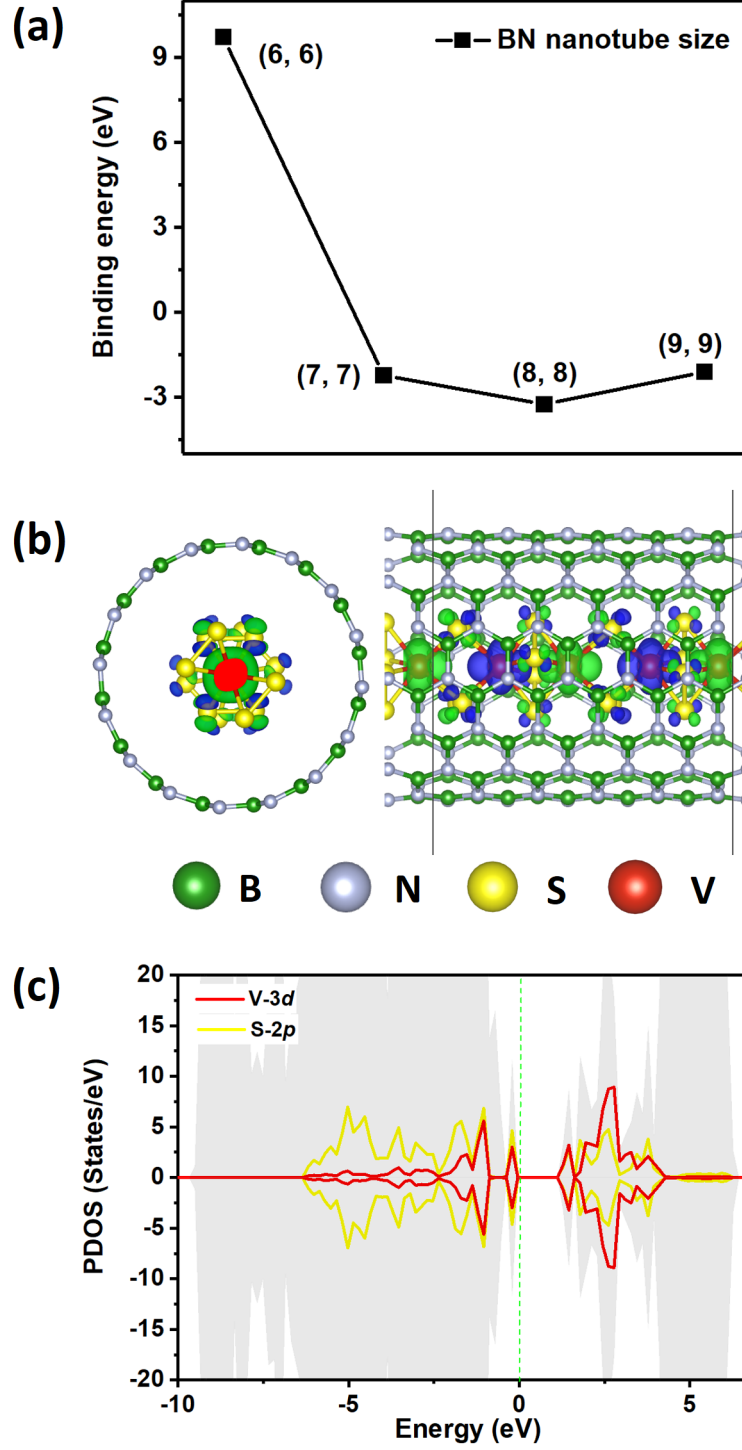


Figure S6: (a) Binding energies E_b of the isolated VS_4 NW inside various BN nanotubes are presented. (b) Spin polarization density of the nanocable. (c) The partial density of states of the nanocable at $PBE + U$ level ($U = 3$). The gray shadow is the total density of states.

2 Structures

VS₄ Bulk

1.0000000000000000
8.2578643546317636 -0.2312003852802180 0.1725788507858386
-1.3475349019652072 8.1504556318164614 -0.1725788507903324
-2.1111532963959965 1.8421889874105739 6.2507753365645335
V S
4 16
Direct
0.1151230690434864 0.3834309663873056 0.1159304648625106
0.8848769169565125 0.6165690056126989 0.8840694901374893
0.3834309713873025 0.1151230670434863 0.3840695351374894
0.6165689966126945 0.8848768749565161 0.6159304818625086
0.3151048190380170 0.8213454567575662 0.5449422841542487
0.5794696678617833 0.0284298544369706 0.2516460605399661
0.6848951379619830 0.1786544802424321 0.4550576978457500
0.0284298494369763 0.5794696678617858 0.2483539114600393
0.6426671395299407 0.6670455141794629 0.9706051672514334
0.1224427794917827 0.1848646593426574 0.4522796726562012
0.8151352596573476 0.8775571625082212 0.9522796636561991
0.9715700925630261 0.4205303761382179 0.7516460875399641
0.4205303601382190 0.9715700625630259 0.7483538844600401
0.3329544588205394 0.3573328244700577 0.4706051412514335
0.8775571905082217 0.8151352856573415 0.5477202723437977
0.1848646713426573 0.1224427884917782 0.0477203183437993
0.3573328264700563 0.3329544458205411 0.0293948367485670
0.1786544762424309 0.6848951439619765 0.0449422891542560
0.6670455401794639 0.6426671125299408 0.5293948407485651
0.8213454947575702 0.3151048500380229 0.9550576878457454

Isolated VS₄ NW

1.0000000000000000
15.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 11.9700000000000006
V S
4 16
Direct
0.5064028705863399 0.5177830768638931 0.0697618377079611
0.5063994270443732 0.5177877508029679 0.8005643430698741
0.5063971228986414 0.5177811664904107 0.3006685393300112
0.5063894863576013 0.5177895819315762 0.5694768028259313
0.3778298259752553 0.5338904808806391 0.1852698247934681
0.4618289930075137 0.6398341217148228 0.1852034921631348
0.6349704802306270 0.5016708602818564 0.1852786467783339
0.5509677867110832 0.3957314350776089 0.1852050705984686
0.5748985261410903 0.4132108392358237 0.4455561301968611
0.4409981125864715 0.4111231557302272 0.4244709869204129
0.4378783638204362 0.6223573257663990 0.4455468278907466
0.5717801832344470 0.6244493306540486 0.4244722489495782
0.5472427615611691 0.6410891327794723 0.6850330622741672
0.6343820984846620 0.5376928741576963 0.6849576315112524
0.4655324352047515 0.3944920090798964 0.6850352028365122
0.3784042744599979 0.4978971666093134 0.6849748048679370
0.5749016617011351 0.4133345099437005 0.9247532002866439
0.4410123053481316 0.4112576323906599 0.9456797329635706
0.4379015766589485 0.6222329084084711 0.9247607846321635
0.5717916539873127 0.6243147792005043 0.9456808744029742