Supplementary Information for

2D Rashba electron gas with large spin splitting in Janus structure of $SnPbO_2$

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Table S1. The energy convergence test for the K-points and Cut-off energy

K-points	Total energy (eV)	Cut-off energy (eV)	Total energy (eV)
10×10×1	-22.39902266	400	-22.43032886
15×15×1	-22.39901985	500	-22.3949235
20×20×1	-22.39901770	600	-22.39902086
25×25×1	-22.39901954	700	-22.40389569
30×30×1	-22.39901688	800	-22.40581925
35×35×1	-22.39901934	900	-22.40599395
40×40×1	-22.39901761	1000	-22.40601808

As shown in Table S1, the energy are converged to 10^{-5} eV level for K-points of 15×15×1 and cut-off energy of 800 eV. Based on this test, the K-points of 30×30×1 and cut-off energy of 800 eV are used in our calculation for sufficient accuracy.

The structure information of $SnPbO_2$ (POSCAR format) we predicted and the input parameters (INCAR format) are given below.

POSCAR:

```
SnPbO2
   1.0
     3.8635      0.00      0.00
     0.00      3.8635      0.00
```

```
      0.00      0.00     22.3589
   Pb    Sn    O
      1       1       2
Direct
  0.0   0.5   0.551617
  0.5   0.0   0.445310
  0.5   0.5   0.496026
  0.0   0.0   0.496026
```

A typical INCAR: (note that some commented tags need to be uncommented when necessary)

INCAR

```
SYSTEM=SnPbO2
  PREC=High
  ENCUT=800
  ISTART=0
  ICHARG=1
  INIWAV=1
  NSW=0
  NELM = 200
  IBRION=-1
  ISIF=0
  EDIFF=1.0E-06
  EDIFFG= -0.001
  ISMEAR=0
  SIGMA = 0.05
  LORBIT=11
  GGA=PE
  #ISPIN=2
#setting for dos
  EMAX=20
  EMIN=-20
  NEDOS=2000
  IVDW=11
    # SOC setting #    uncomment when use
    #LSORBIT=.TURE.
    #SAXIS= 0 0 1
#MD setting    #    uncomment when use
  #POTIM=3
  #SMASS=2
  #TEBEG=300
  #TEEND=300
```