# Zigzag Antiferromagnetic Property of Two-dimensional $NiPX_3$ (X=S/Se) in Pristine Structure and Janus Phase

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## I. SUPPLEMENTARY INFORMATION

TABLE S1: The $p$-orbital electron numbers $N$ ($e$) of chalcogen element in an energy range from -0.5 eV to the Fermi level for 2D $NiPX_3$ and $NiPS_{3/2}Se_{3/2}$, respectively. Here only the electrons in spin-up or spin-down channel were counted, for simplicity, the $N$ was taken to be one-half of the actual number of pristine strcutre in order to compare with that of Janus structure.

| | Element | $p_x$ | $p_y$ | $p_z$ | $N$ |
|---|---|---|---|---|---|
| $NiPS_3$ | S | 0.58 | 0.57 | 0.67 | 1.62 |
| $NiPSe_3$ | Se | 0.64 | 0.58 | 0.74 | 1.96 |
| $NiPS_{3/2}Se_{3/2}$ | S | 0.27 | 0.26 | 0.41 | 0.94 |
| | Se | 0.88 | 0.78 | 0.67 | 2.33 |

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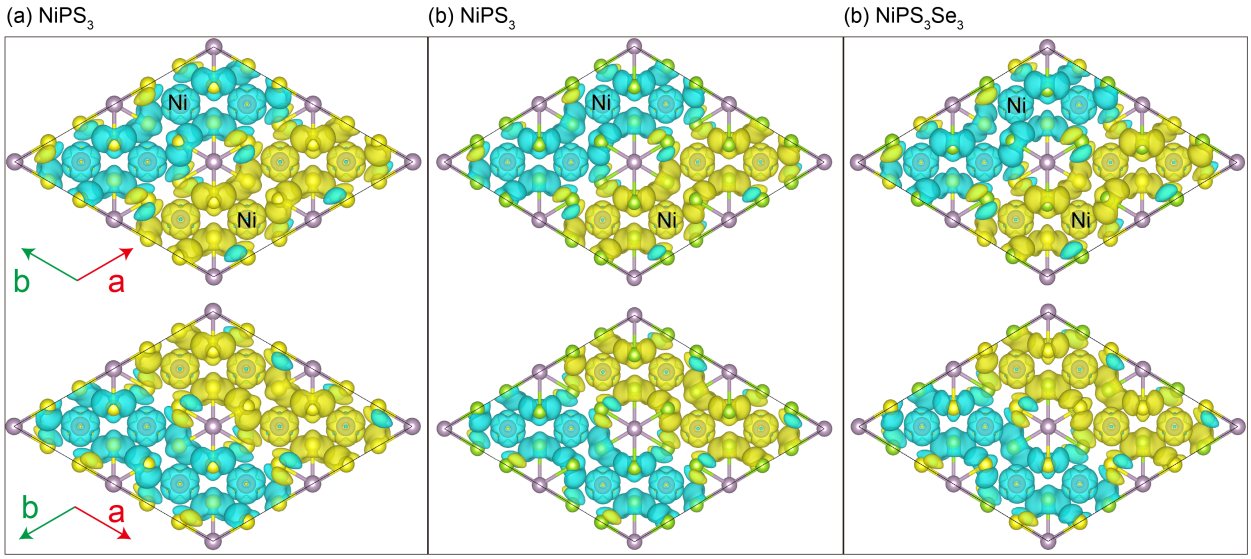


FIG. S1: Spin charge density maps of 2D (a) $NiPS_3$, (b) $NiPSe_3$ and (c) $NiPS_{3/2}Se_{3/2}$ in top and bottom views, respectively. The isosurface is $2 \times 10^{-3}$ e/$A^{-3}$ with spin up and down electrons indicated by blue and yellow colors, respectively.

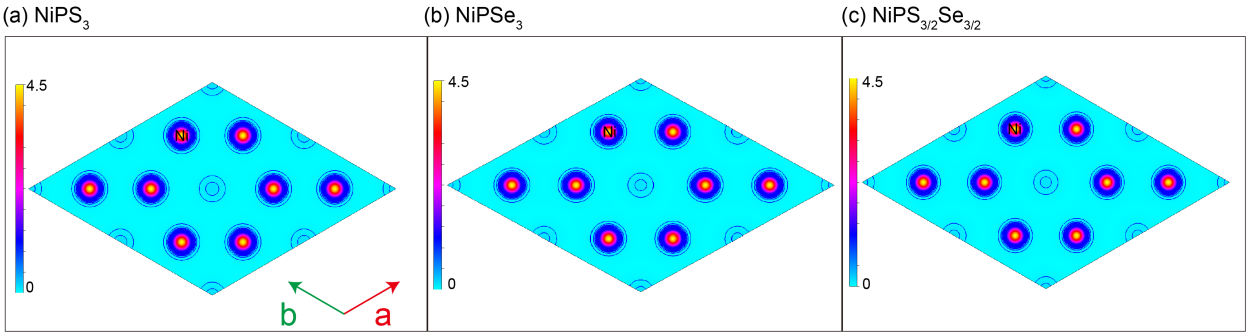


FIG. S2: Charge density maps in the Ni hexagonal slide of 2D (a) $NiPS_3$, (b) $NiPSe_3$ and (c) $NiPS_{3/2}Se_{3/2}$, respectively. The blue contour line indicates a density of $5 \times 10^{-2}$ e/$A^{-2}$, and the color bar represents the range of charge density values.

NiPS3
1.000000000000
5.062572452064177037 2.9228775679912359 0.0000000000000000
-5.062572452064177037 2.9228775679912359 0.0000000000000000
0.000000000000000000 0.0000000000000000 25.2993762993762985
Ni P S
2 2 6
Direct
0.6666666666666643 0.3333333333333357 0.5000000000000000
0.3333333333333357 0.6666666666666643 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.4569350031289284
0.0000000000000000 0.0000000000000000 0.5430649968710712
0.6605882071972612 -0.0000000000000000 0.4380692387217583
0.0000000000000000 0.6605882071972612 0.4380692387217583
0.3394117928027458 0.3394117928027458 0.4380692387217583
0.3394117928027458 0.0000000000000000 0.5619307612782413
0.0000000000000000 0.3394117928027458 0.5619307612782413
0.6605882071972612 0.6605882071972612 0.5619307612782413

NiPSe3
1.00000000000
5.3520126650200292 3.0899859528555997 0.0000000000000000
-5.3520126650200292 3.0899859528555997 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.2999999999999999
Ni P Se
2 2 6
Direct
0.6666666666666643 0.3333333333333357 0.5000000000000000
0.3333333333333357 0.6666666666666643 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.4564460404938710
0.0000000000000000 0.0000000000000000 0.5435539595061291
0.6524128982467414 0.0000000000000000 0.4353310351754001
0.0000000000000000 0.6524128982467414 0.4353310351754001
0.3475871017532653 0.3475871017532653 0.4353310351754001
0.3475871017532653 0.0000000000000000 0.5646689648246002
0.0000000000000000 0.3475871017532653 0.5646689648246002
0.6524128982467414 0.6524128982467414 0.5646689648246002

NiPSSe
1.00000000000
5.162560889267108 2.9806059191261980 0.0000000000000000
-5.162560889267108 2.9806059191261980 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.30000000000000
Ni P S Se
2 2 3 3
Direct
0.6666666666666643 0.3333333333333357 0.5000000000000000
0.3333333333333357 0.6666666666666643 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.4619978812302245
0.0000000000000000 0.0000000000000000 0.5488881678503379
0.6643253169064418 0.0000000000000000 0.4437671927009335
0.0000000000000000 0.6643253169064418 0.4437671927009335
0.3356746830935660 0.3356746830935660 0.4437671927009335
0.3624953204439907 0.0000000000000000 0.5669451646546656
0.0000000000000000 0.3624953204439907 0.5669451646546656
0.6375046795560160 0.6375046795560160 0.5669451646546656