# Supporting Information for

## Two-dimensional semiconducting with high stability and electron mobility in group-11 chalcogenide compounds: MNX (M = Cu, Ag, Au; N = Cu, Ag, Au; X = S, Se, Te; M≠N)

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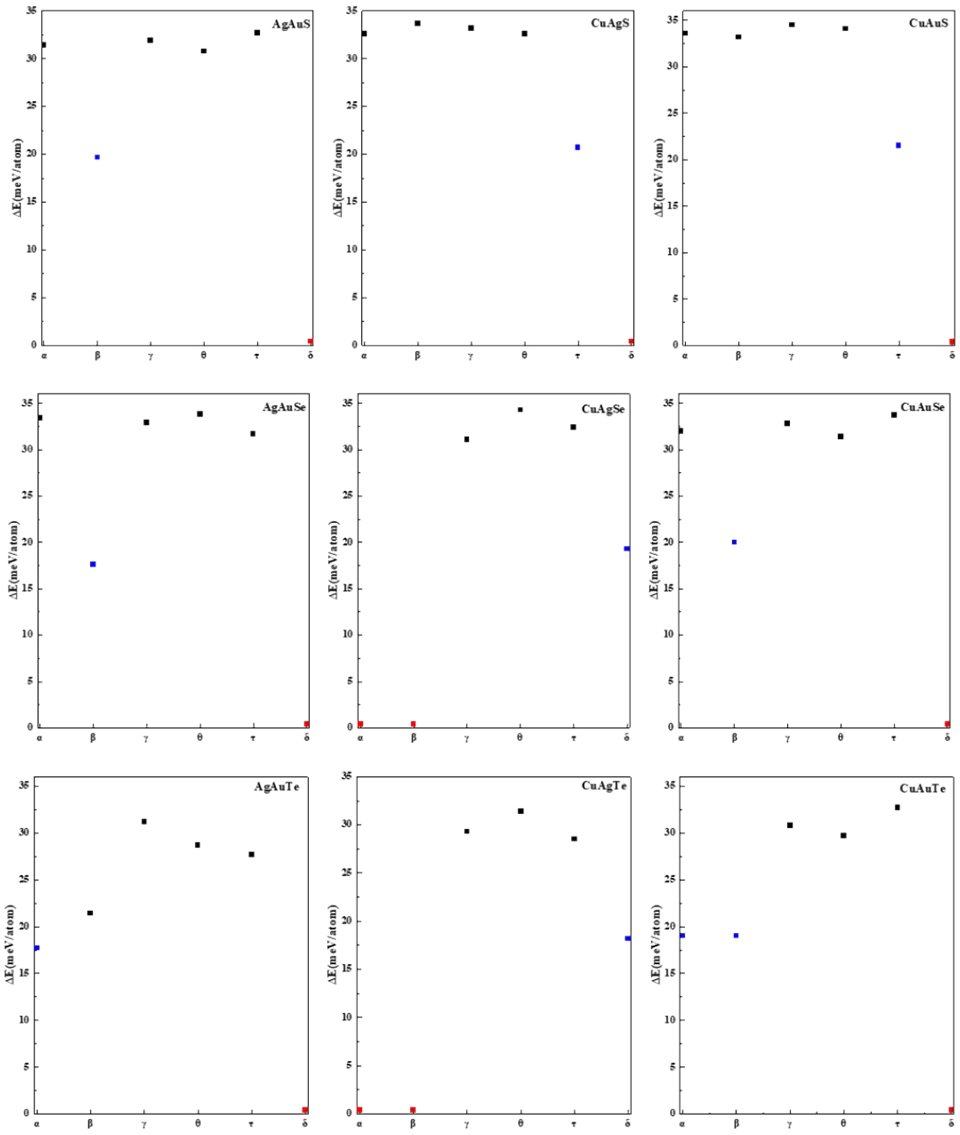


**Figure S1. The relative energy of the nine MNX (M = Cu, Ag, Au; M = Cu, Ag, Au; X = S, Se, Te; M≠N) monolayers with six allotropes , the phase with the lowest energy is shown in red, and the phase with the next lowest energy is shown in blue.**

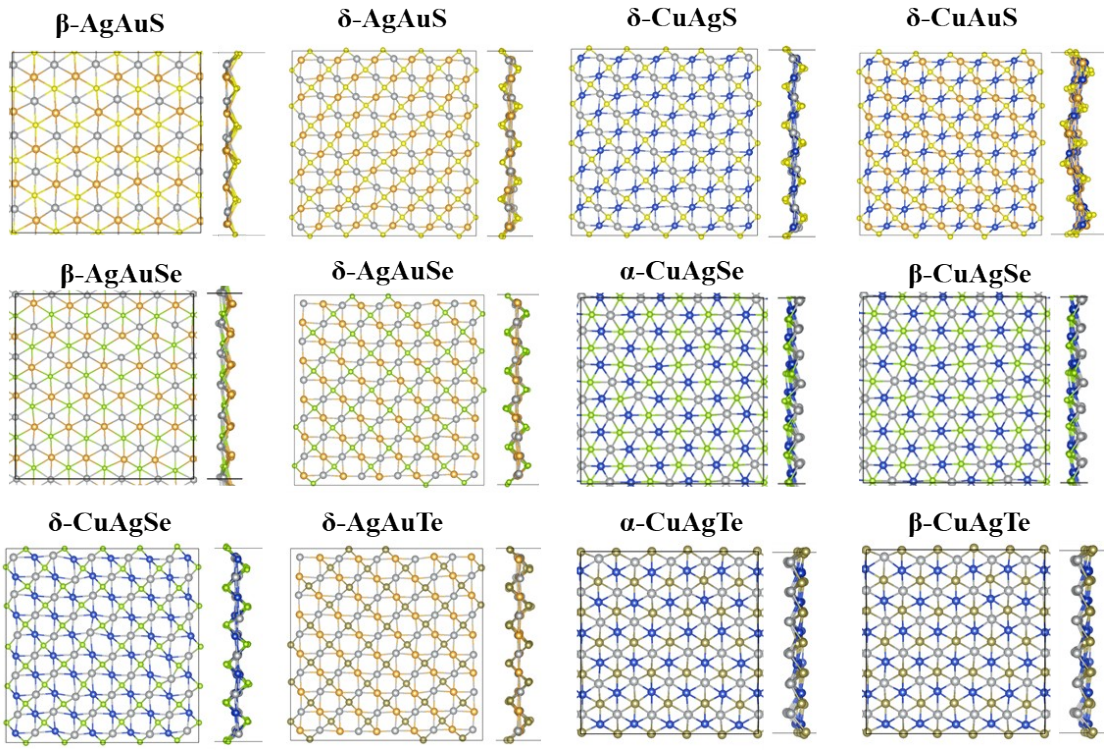


**Figure S2. Top and side views of the snapshots of the atomic configurations of the MNX monolayers taken from FPMD simulations carried out at 300 K for 10 ps.**

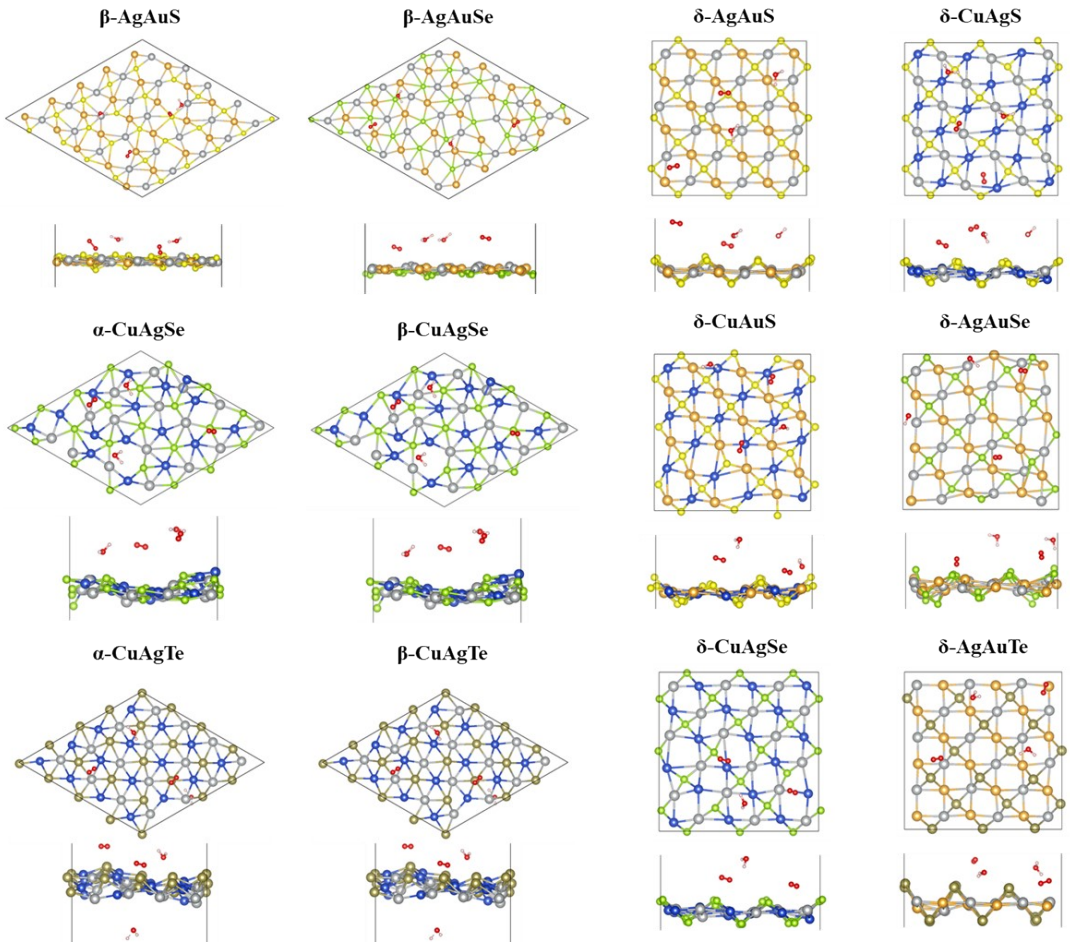


**Figure S3. The FPMD simulation was performed on the monolayer MNX with two $O_2$ and two $H_2O$ molecules adsorbed at 300 K for 5 ps.**

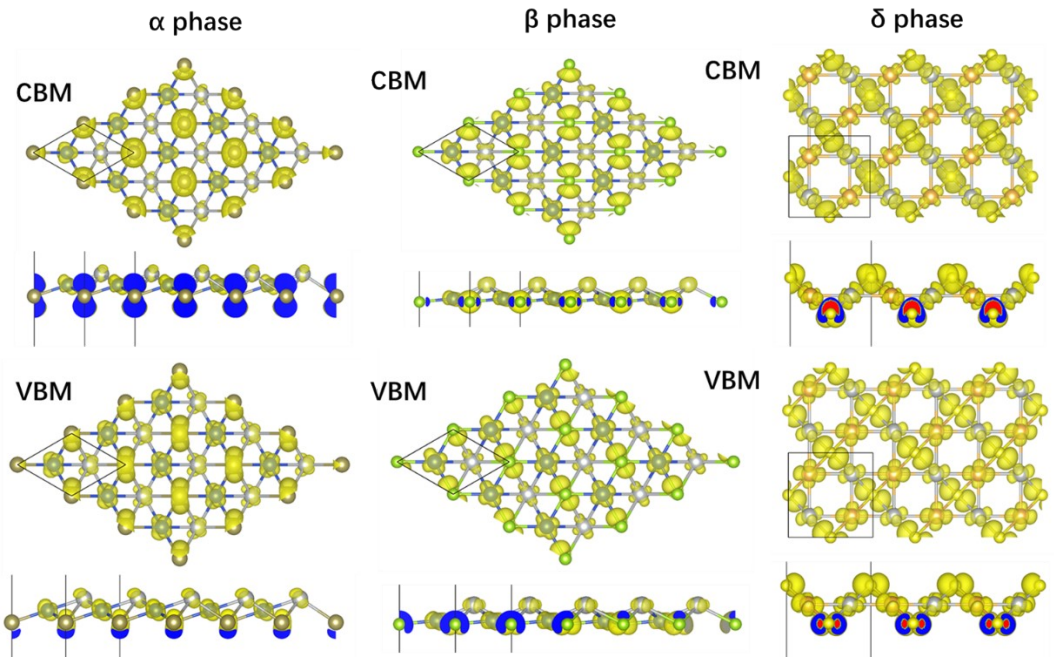


**Figure S4. The CBM and VBM electron density of the MNX monolayer (α, β, δ phases)**

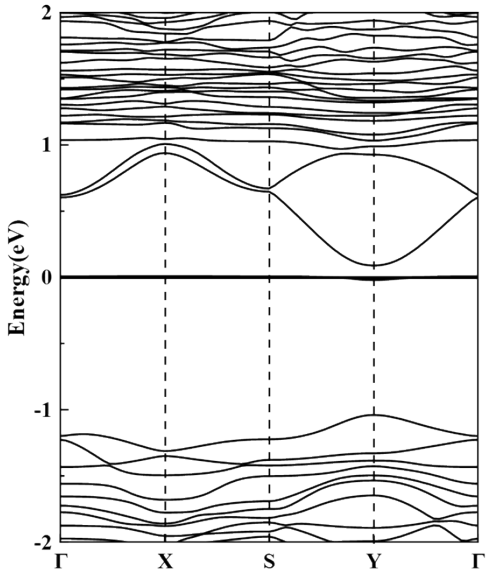


**Figure S5. The band structure of the δ-phase MNX monolayer adsorbed by $O_2$ and $H_2O$.**

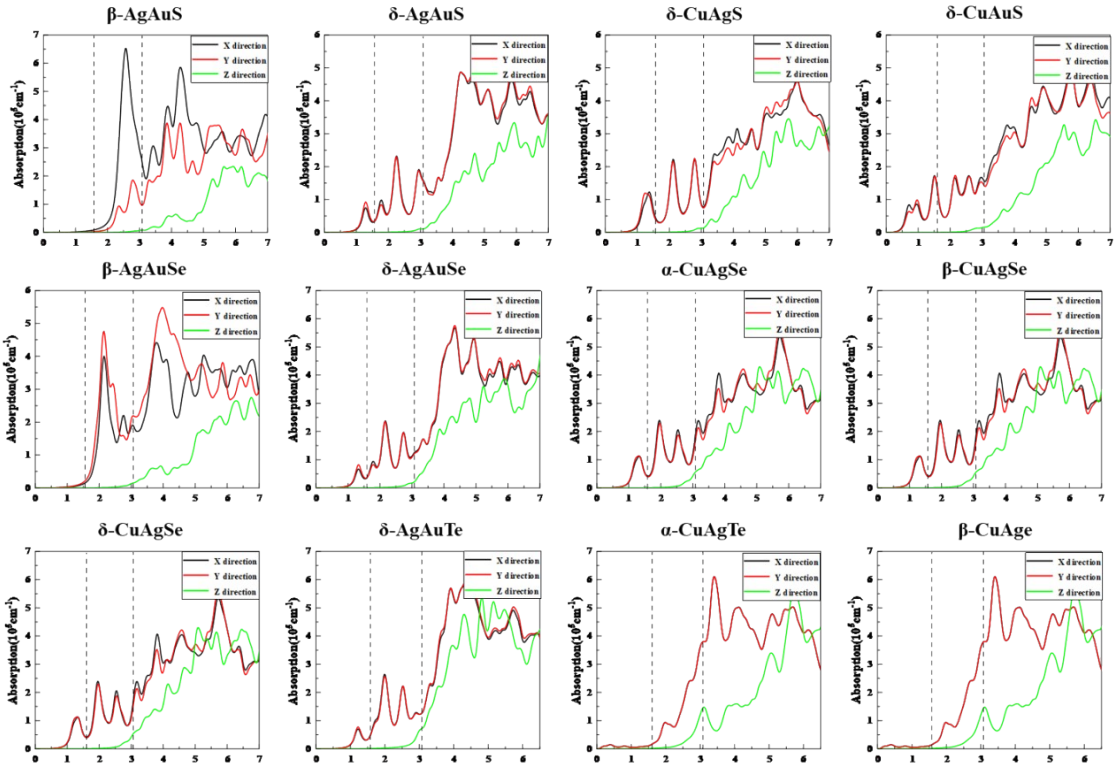


**Figure S6. Light absorption of the MNX monolayer. The light absorption transformed by the xx, yy and zz components of the imaginary part of the dielectric constant tensor are represented by black, red and green respectively. The part between the two dotted lines represents the visible light area.**

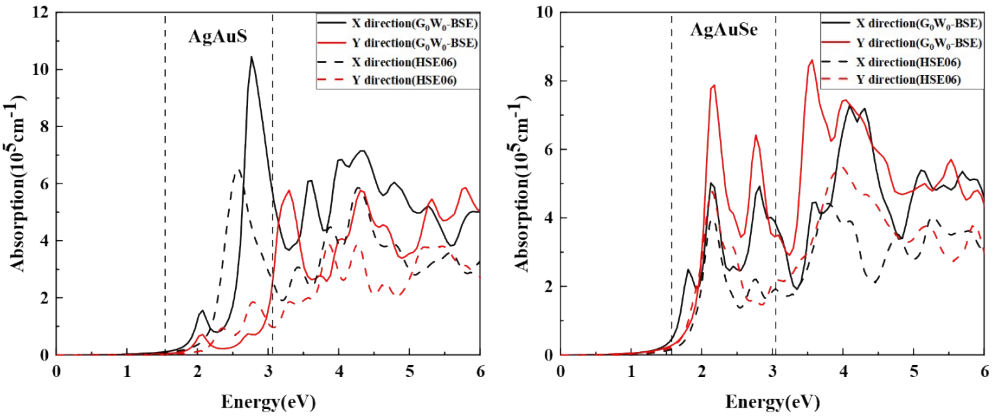


**Figure S7. Light absorption of the β-AgAuS，β-AgAuSe monolayer at $G_0W_0$+BSE level without SOC. The light absorption transformed by the xx and yy components of the imaginary part of the dielectric constant tensor are represented by black,**

**red respectively. The part between the two dotted lines represents the visible light area.**

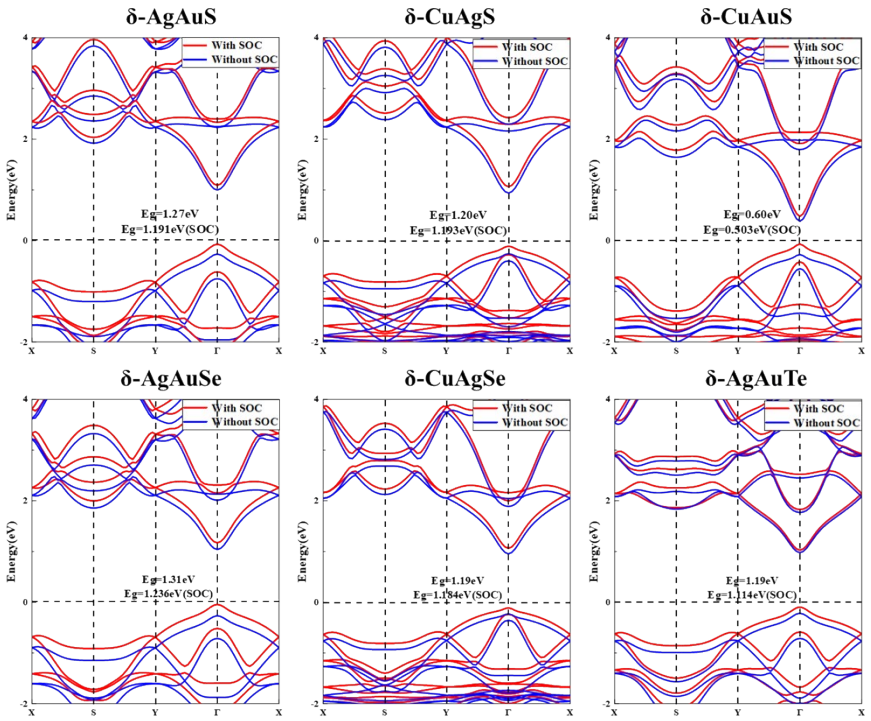


**Figure S8. Band structures without and with SOC effect of δ-MNX monolayer.**

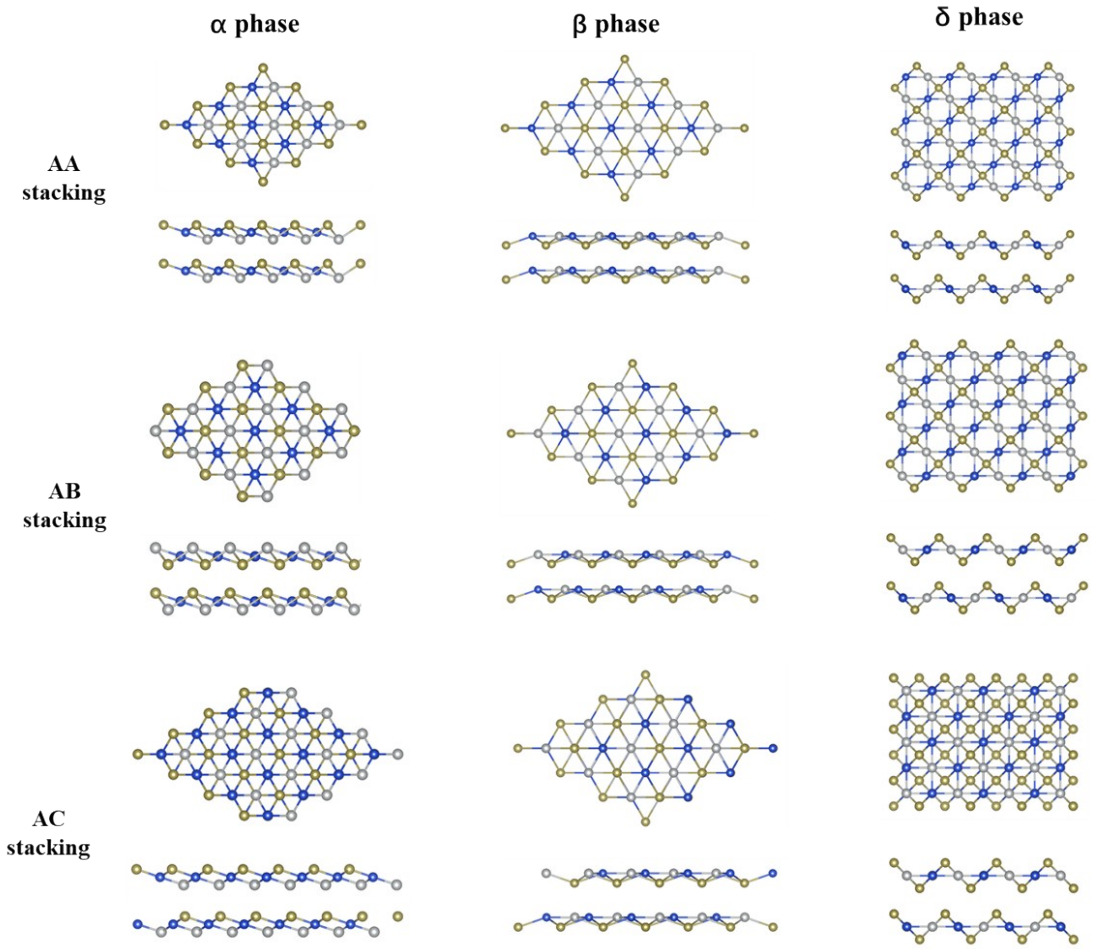


**Figure S9. The structure optimized of the two-layer MNX system with different stacking methods.**

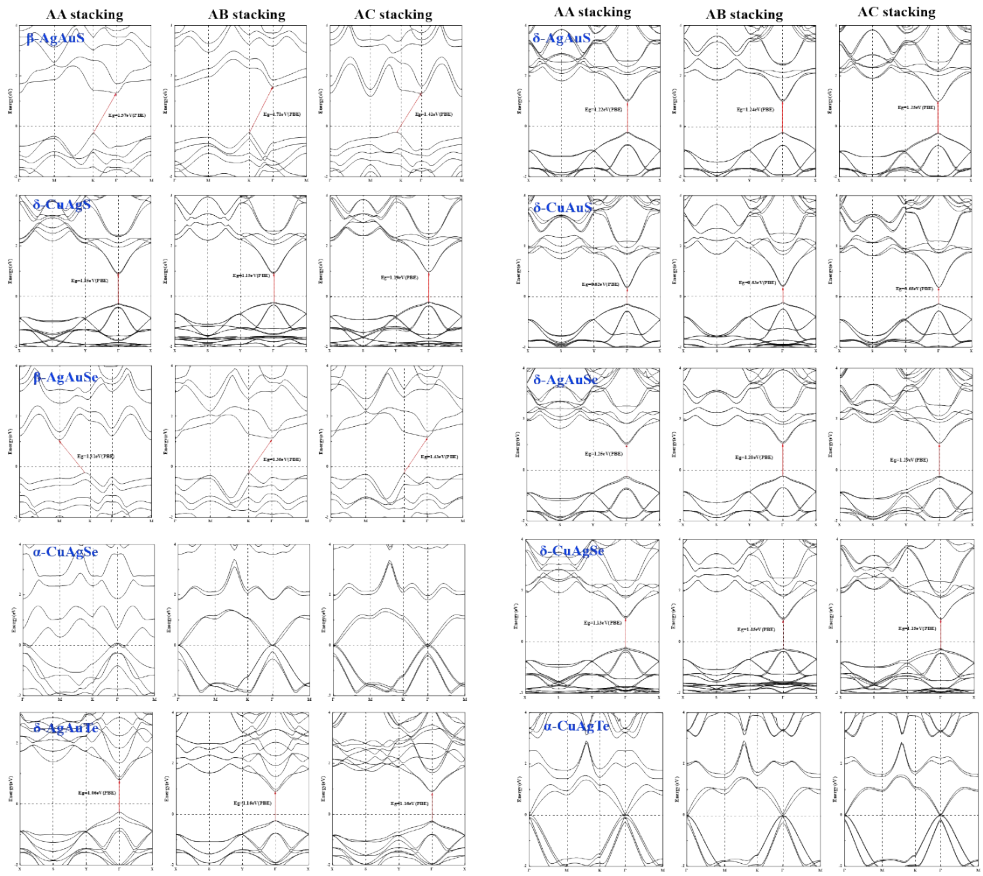


**Figure S10. The band structures of a two-layer MNX system with different stacking methods calculated based on the PBE function.**

**Table S1. Structural parameters and Electronic Band gaps of the β-AgAuS, δ-AgAuS, δ-CuAgS, δ-CuAuS, β-AgAuSe, δ-AgAuSe, α-CuAgSe, δ-CuAgSe, δ-AgAuTe and α-CuAgTe monolayers. a and b are the lattice parameters; h denotes the thickness of these Group-11-chalcogenide monolayers; CBM and VBM stand for the conduction band minimum and the valence band maximum on the theoretical level of HSE06, respectively.**

| phases | lattice parameters | h (Å) | CBM | VBM | Band gaps(eV) HSE06 |
|---|---|---|---|---|---|
| β-AgAuS | a = b = 4.45 Å | 1.58 | 2.2046 | -0.3629 | 2.5675(I) |
| δ-AgAuS | a = b = 5.85 Å | 3.63 | 1.6922 | -0.2701 | 1.9623(D) |
| δ-CuAgS | a = b = 5.55 Å | 3.07 | 1.8751 | -0.2383 | 2.1134(D) |
| δ-CuAuS | a = b = 5.47 Å | 2.88 | 1.1677 | -0.2406 | 1.4083(D) |
| β-AgAuSe | a = b = 4.78 Å | 1.37 | 2.4862 | -0.1602 | 2.6464(I) |
| δ-AgAuSe | a = b = 5.87 Å | 2.98 | 1.7307 | -0.2447 | 1.9754(D) |
| α-CuAgSe | a = b = 4.27 Å | 1.26 | 0.3065 | -0.3107 | 0.6172(D) |
| β-CuAgSe | a = b = 4.27 Å | 1.26 | 0.3065 | -0.3107 | 0.6172(D) |
| δ-CuAgSe | a = b = 5.52 Å | 3.52 | 1.7949 | -0.2459 | 2.0408(D) |
| δ-AgAuTe | a = b = 5.91 Å | 3.67 | 1.5556 | -0.2127 | 1.7683(D) |
| α-CuAgTe | a = b = 4.32 Å | 1.65 | 0.4760 | -0.1309 | 0.6068(D) |
| β-CuAgTe | a = b = 4.32 Å | 1.65 | 0.4760 | -0.1309 | 0.6068(D) |

**Table S2. The formation energy ($E_f$ in meV/atom) of MNX to ascertain the**

**thermodynamic stability.**

| Materials | $E_f$(meV) |
|---|---|
| **β-AgAuS** | -40.02 |
| **δ-AgAuS** | -17.54 |
| **δ-CuAgS** | -31.84 |
| **δ-CuAuS** | -26.09 |
| **β-AgAuSe** | -22.16 |
| **δ-AgAuSe** | -22.23 |
| **α-CuAgSe** | -13.98 |
| **δ-CuAgSe** | -23.97 |
| **δ-AgAuTe** | -9.98 |
| **α-CuAgTe** | -28.34 |

**Table S3. The binding energy ($E_b$ in meV/atom) of the two-layer system with different stacking modes was calculated on the theoretical level of PBE+D2. The $E_B$ is defined as the energy sum of the two corresponding MNX monolayers minus the total energy of the fully relaxed MNX bilayer system.**

| | AA Stacking | AB Stacking | AC Stacking |
|---|---|---|---|
| | $E_b$ | $E_b$ | $E_b$ |
| **β-AgAuS** | 6.47 | 40.72 | 48.10 |
| **δ-AgAuS** | 25.65 | 204.53 | 19.91 |
| **δ-CuAgS** | 24.97 | 166.70 | 15.53 |
| **δ-CuAuS** | 18.93 | 297.31 | 15.45 |
| **β-AgAuSe** | 15.03 | 55.78 | 14.43 |
| **δ-AgAuSe** | 27.92 | 146.27 | 20.41 |
| **α-CuAgSe** | 31.83 | 9.82 | 16.54 |
| **δ-CuAgSe** | 24.77 | 87.76 | 10.89 |
| **δ-AgAuTe** | 48.70 | 71.23 | 25.02 |
| **α-CuAgTe** | 49.18 | 7.88 | 46.23 |

**Table S4. Elastic constants ($C_{ij}$, N/m), Layer modulus (γ, N/m), Young's modules (Y, N/m), Poisson's ratio (υ) of ten low-lying allotropes of 2D MNX nanosheets.**

| Phase | C11 | C22 | C12 | C66 | γ | G2D(N/m) | Young modulus (N/m) | | Poisson's ratio | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | $Y_x$ | $Y_y$ | $\upsilon_x$ | $\upsilon_y$ |
| **β-AgAuS** | 21.9 | 15.4 | 2.4 | 9.8 | 10.5 | 9.8 | 21.5 | 14.8 | 0.1589 | 0.1096 |
| **δ-AgAuS** | 28.7 | 28.3 | 6.8 | 10.9 | 17.6 | 10.9 | 27.1 | 26.5 | 0.2428 | 0.2369 |
| **δ-CuAgS** | 24.5 | 23.9 | 2.6 | 12.0 | 13.4 | 12.0 | 24.2 | 23.6 | 0.1088 | 0.1061 |
| **δ-CuAuS** | 32.2 | 31.3 | 5.1 | 13.6 | 18.4 | 13.6 | 31.3 | 30.5 | 0.1629 | 0.1584 |
| **β-AgAuSe** | 31.4 | 30.9 | 12.3 | 9.6 | 21.7 | 9.6 | 26.5 | 16.1 | 0.3981 | 0.3917 |
| **δ-AgAuSe** | 25.4 | 25.0 | 5.3 | 10.0 | 15.3 | 10.0 | 24.3 | 23.9 | 0.2120 | 0.2087 |
| **α-CuAgSe** | 33.3 | 32.7 | 7.6 | 12.9 | 20.3 | 7.6 | 31.5 | 31.0 | 0.2324 | 0.2282 |
| **δ-CuAgSe** | 16.7 | 16.7 | 2.3 | 7.2 | 9.5 | 7.2 | 16.4 | 16.4 | 0.1377 | 0.1377 |
| **δ-AgAuTe** | 21.5 | 21.9 | 5.5 | 8.0 | 13.6 | 8.0 | 20.1 | 20.5 | 0.2511 | 0.2571 |
| **α-CuAgTe** | 31.0 | 31.5 | 7.8 | 11.6 | 19.5 | 11.6 | 29.1 | 29.5 | 0.2476 | 0.2516 |

## The Atomic Coordinates of MNX Monolayer

α-phase
1.0
2.9900000095 0.0000000000 0.0000000000
1.4950000048 2.5894159656 0.0000000000
0.0000000000 0.0000000000 20.0000000000
M N X
1 1 1
Cartesian
1.494850480 0.863052327 9.598399997
0.000000000 0.000000000 10.058399439
2.989970158 1.726260076 9.138399959

β-phase
1.0
7.0000000000 0.0000000000 0.0000000000

3.5000000000 6.0621778265 0.0000000000
0.0000000000 0.0000000000 20.0000000000
M N X
1 1 1
Cartesian
0.000000000 0.000000000 8.885800242
3.499649733 2.020523836 11.085799932
7.000035256 4.041472239 11.085799932

γ-phase
1.0
5.0000000000 0.0000000000 0.0000000000
2.5000000000 4.3301270189 0.0000000000
0.0000000000 0.0000000000 20.0000000000
M N X
1 1 1
Cartesian
0.000000000 0.000000000 8.885800242
2.499749959 1.443231311 10.629800558
2.499749959 1.443231311 7.141200304

θ-phase
1.0
6.0000000000 0.0000000000 0.0000000000
0.0000000000 4.0000000000 0.0000000000
0.0000000000 0.0000000000 20.0000000000
M N X
1 1 1
Cartesian
0.000000000 0.000000000 10.079400539
1.998000026 2.000000000 10.079400539
4.001999974 2.000000000 10.079400539

γ-phase
1.0
8.0000000000 0.0000000000 0.0000000000
0.0000000000 8.0000000000 0.0000000000
0.0000000000 0.0000000000 20.0000000000
M N X
4 4 4
Cartesian

| | | |
|---|---|---|
| 4.000000000 | 4.000000000 | 6.000000238 |
| 4.000000000 | 0.000000000 | 6.000000238 |
| 0.000000000 | 0.000000000 | 11.000000238 |
| 0.000000000 | 4.000000000 | 11.000000238 |
| 2.000000000 | 0.000000000 | 8.500000238 |
| 6.000000000 | 0.000000000 | 8.500000238 |
| 0.000000000 | 2.000000000 | 8.500000238 |
| 0.000000000 | 6.000000000 | 8.500000238 |
| 4.000000000 | 6.000000000 | 8.500000238 |
| 4.000000000 | 2.000000000 | 8.500000238 |
| 2.000000000 | 4.000000000 | 8.500000238 |
| 6.000000000 | 4.000000000 | 8.500000238 |

δ-phase

1.0

| | | |
|---|---|---|
| 5.7480001450 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 5.7480001450 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 20.0000000000 |

| M | N | X |
|---|---|---|
| 2 | 2 | 2 |

Cartesian

| | | |
|---|---|---|
| 1.437172539 | 4.311229998 | 8.156599998 |
| 4.310827777 | 1.436827619 | 8.156599998 |
| 1.437172539 | 1.436827619 | 8.156599998 |
| 4.310827777 | 4.311229998 | 8.156599998 |
| 2.874000072 | 0.000000000 | 9.684000015 |
| 0.000000000 | 2.874000072 | 6.629599929 |