TABLE I: Bond distances (nm) and dihedral angles (°) between two planes (passing through the elements of groups as given in column four and column nine) of the III-IV-V nanosheet.

| System | Bond | Length | Planes | angle | System | Bond | Length | Planes | angle |
|---|---|---|---|---|---|---|---|---|---|
| $BC_2N$ | BN | 0.144 | 444-443 | 0 | $BC_2P$ | BP | 0.174 | 444-443 | 0 |
| | CC | 0.141 | 353-334 | 0 | | CC | 0.152 | 353-334 | 0 |
| | BC | 0.151 | 444-445 | 0 | | BC | 0.151 | 444-445 | 0 |
| | CN | 0.137 | 535-554 | 0 | | CP | 0.173 | 535-554 | 0 |
| $BC_2As$ | BAs | 0.182 | 444-443 | 0 | $AlSi_2As$ | AlAs | 0.235 | 444-443 | 14.5 |
| | CC | 0.154 | 353-334 | 0 | | SiSi | 0.225 | 353-334 | 17.0 |
| | BC | 0.150 | 444-445 | 0 | | AlSi | 0.237 | 444-445 | 21.7 |
| | CAs | 0.184 | 535-554 | 0 | | SiAs | 0.228 | 535-554 | 24.1 |
| $AlSi_2Sb$ | AlSb | 0.254 | 444-443 | 11.4 | $GaSi_2P$ | GaP | 0.225 | 444-443 | 18.9 |
| | SiSi | 0.228 | 353-334 | 21.8 | | SiSi | 0.225 | 353-334 | 13.9 |
| | AlSi | 0.237 | 444-445 | 18.8 | | GaSi | 0.231 | 444-445 | 17.0 |
| | SiSb | 0.25 | 535-554 | 28.5 | | SiP | 0.217 | 535-554 | 12.5 |
| $GaSi_2As$ | GaAs | 0.235 | 444-443 | 18.5 | $GaSi_2Sb$ | GaSb | 0.251 | 444-443 | 16.4 |
| | SiSi | 0.226 | 353-334 | 20.4 | | SiSi | 0.230 | 353-334 | 21.5 |
| | GaSi | 0.231 | 444-445 | 20.9 | | GaSi | 0.232 | 444-445 | 22.2 |
| | SiAs | 0.228 | 535-554 | 22.7 | | SiSb | 0.250 | 535-554 | 26.9 |
| $GaGe_2P$ | GaP | 0.228 | 444-443 | 28.8 | $GaGe_2As$ | GaAs | 0.237 | 444-443 | 26.6 |
| | GeGe | 0.235 | 353-334 | 18.0 | | GeGe | 0.237 | 353-334 | 22.9 |
| | GaGe | 0.238 | 444-445 | 23.8 | | GaGe | 0.238 | 444-445 | 25.7 |
| | GeP | 0.224 | 535-554 | 13.1 | | GeAs | 0.236 | 535-554 | 21.4 |
| $GaGe_2Sb$ | GaSb | 0.254 | 444-443 | 25.6 | $AlGe_2Sb$ | AlSb | 0.255 | 444-443 | 24.8 |
| | GeGe | 0.240 | 353-334 | 22.9 | | GeGe | 0.24 | 353-334 | 28.1 |
| | GaGe | 0.239 | 444-445 | 27.5 | | AlGe | 0.242 | 444-445 | 26.1 |
| | GeSb | 0.256 | 535-554 | 25.4 | | GeSb | 0.256 | 535-554 | 25.0 |
| $InSn_2As$ | InAs | 0.259 | 444-443 | 31.5 | $InSn_2Sb$ | InSb | 0.275 | 444-443 | 29.4 |
| | SnSn | 0.273 | 353-334 | 22.9 | | SnSn | 0.275 | 353-334 | 23.3 |
| | InSn | 0.276 | 444-445 | 27.0 | | InSn | 0.276 | 444-445 | 29.0 |
| | SnAs | 0.254 | 535-554 | 18.6 | | SnSb | 0.254 | 535-554 | 22.9 |

TABLE II: Comparison of the binding energy, BE (eV/atom) and electronic band gap, $E_g$ (eV) of various IV-IV, III-V and III-IV-V nanosheets as calculated using LDA, GGA and hybrid functionals. SM is the abbreviation used for denoting the semi-metallic electronic states. The point in the K-mesh where direct transition is found to be the smallest is given in the bracket.

| System | BE | | | $E_g$ | | |
|---|---|---|---|---|---|---|
| | GGA | LDA | HSE06 | GGA | LDA | HSE06 |
| C | -7.503 | -8.907 | -7.66 | SM | SM | SM |
| Si | -2.835 | -4.576 | -3.86 | SM | SM | SM |
| Ge | -2.359 | -3.940 | -3.19 | SM | SM | SM |
| Sn | -1.322 | -2.994 | -2.23 | SM | SM | SM |
| BN | -6.648 | -7.964 | -6.847 | 4.78 | 4.58 $(K-K)$ | 6.284 |
| BP | -4.150 | -5.707 | -4.099 | 1.16 | 0.81 $(K-K)$ | 1.389 |
| AlAs | -2.154 | -3.865 | -3.191 | 1.75 | 1.82 | 2.814 |
| AlSb | -1.576 | -3.414 | -2.763 | 1.37 | 1.51 | 2.089 |
| GaP | -2.159 | -3.783 | -3.024 | 1.67 | 1.85 | 2.927 |
| GaAs | -1.893 | -3.498 | -2.734 | 1.13 | 1.31 $(\Gamma-\Gamma)$ | 2.28 |
| GaSb | -1.315 | -3.053 | -2.417 | 0.92 | 0.98 | 1.37 |
| InAs | -1.256 | -3.218 | -2.458 | 0.82 | 0.84 $(\Gamma-\Gamma)$ | 1.677 |
| InSb | -0.870 | -2.958 | -2.236 | 0.72 | 0.77 $(\Gamma-\Gamma)$ | 1.521 |
| $BC_2N$ | -6.843 | -8.203 | -7.011 | 1.582 | 1.589 $(\Gamma-\Gamma)$ | 2.23 |
| $BC_2P$ | -5.494 | -6.814 | -4.473 | 0.090 | 0.112 $(\Gamma-\Gamma)$ | 0.371 |
| $AlSi_2As$ | -2.398 | -4.122 | -3.408 | 0.560 | 0.568 $(\Gamma-\Gamma)$ | 0.821 |
| $AlSi_2Sb$ | -2.087 | -3.874 | -3.168 | 0.517 | 0.535 $(\Gamma-\Gamma)$ | 0.731 |
| $GaSi_2P$ | -2.463 | -4.147 | -3.390 | 0.731 | 0.758 | 1.061 |
| $GaSi_2As$ | -2.308 | -3.990 | -3.222 | 0.693 | 0.736 | 0.918 |
| $GaSi_2Sb$ | -2.033 | -3.778 | -3.025 | 0.527 | 0.589 | 0.806 |
| $GaGe_2P$ | -2.205 | -3.818 | -3.053 | 0.559 | 0.609 $(\Gamma-\Gamma)$ | 0.894 |
| $GaGe_2As$ | -2.079 | -3.685 | -2.896 | 0.576 | 0.621 $(\Gamma-\Gamma)$ | 0.873 |
| $GaGe_2Sb$ | -1.845 | -3.510 | -2.736 | 0.539 | 0.570 $(\Gamma-\Gamma)$ | 0.764 |
| $AlGe_2Sb$ | -1.894 | -3.607 | -2.881 | 0.476 | 0.536 $(K-K)$ | 0.707 |
| $InSi_2As$ | -2.02 | -3.788 | -3.02 | 0.33 | 0.39$(\Gamma-\Gamma)$ | 0.57 |
| $InSi_2Sb$ | -1.91 | -3.46 | -2.87 | 0.06 | 0.07 $(\Gamma-\Gamma)$ | 0.13 |
| $InGe_2As$ | -1.78 | -3.28 | -2.78 | 0.49 | 0.58 $(\Gamma-\Gamma)$ | 0.88 |
| $InGe_2Sb$ | -1.57 | -3.07 | -2.57 | 0.09 | 0.11 $(\Gamma-\Gamma)$ | 0.20 |
| $InSn_2As$ | -1.232 | -2.952 | -2.514 | 0.173 | 0.385 $(\Gamma-\Gamma)$ | 0.693 |
| $InSn_2Sb$ | -1.068 | -2.766 | -2.419 | 0.426 | 0.449 $(\Gamma-\Gamma)$ | 0.647 |