Supplementary information for

# Structural stability of single-layer $PdSe_2$ with pentagonal puckered morphology and its nanotubes

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Optimized parameters of 2D unit cells studied in this work:

**1. $PdSe_2$**

```
      5.7207007408       0.0000000000       0.0000000000
      0.0000000000       5.9371080399       0.0000000000
      0.0000000000       0.7172031667      17.4304643462
  Pd   Se
   2    4
Direct
    0.000088930        0.999949813        0.499878228
    0.499911100        0.499949783        0.499878228
    0.107548133        0.624555349        0.455207258
    0.892290294        0.375494838        0.544535458
    0.607709706        0.875494838        0.544535458
    0.392451882        0.124555379        0.455207258
```

**2. Penta-graphene**

```
   3.6250998974    0.0000000000    0.0000000000
   0.0000000000    3.6250998974    0.0000000000
   0.0000000000    0.0000000000   17.6223030090
  C
  6
Direct
   0.000351875     0.000351821     0.500000119
   0.130876765     0.630876839     0.534694076
   0.500351787     0.500351906     0.500000119
   0.869826376     0.369826376     0.534694076
   0.630877018     0.869826496     0.465306133
   0.369826555     0.130876929     0.465306133
```

**3. penta-$AlN_2$**

```
   4.4237780571    0.0000000000    0.0000000000
   0.0000000000    4.4237780571    0.0000000000
   0.0000000000    0.0000000000   21.9519100189
  N   Al
  4   2
Direct
   0.108521663     0.608521640     0.472408473
   0.891478360     0.391478330     0.472408473
   0.608521640     0.891478360     0.527591527
   0.391478330     0.108521663     0.527591527
   0.500000000     0.500000000     0.500000000
   0.000000000     0.000000000     0.500000000
```

**4. penta-$CN_2$**

```
   3.3091783524    0.0000000000    0.0000000000
   0.0000000000    3.3091783524    0.0000000000
   0.0000000000    0.0000000000   18.4928646088
  C   N
  2   4
Direct
   0.999400258     0.999380410     0.449308753
   0.499380440     0.499400288     0.449308753
   0.653927088     0.844677031     0.490735918
   0.344677001     0.153927088     0.490735918
   0.844701827     0.344701797     0.407954723
   0.153913394     0.653913379     0.407955885
```

**5. penta-$B_2C$**

```
    3.9317550659    0.0000000000    0.0000000000
    0.0000000000    3.9317550659    0.0000000000
    0.0000000000    0.0000000000   17.2564105988
  B   C
  4   2
Direct
    0.653933644     0.844361067     0.480494767
    0.344361097     0.153933629     0.480494767
    0.845774293     0.345774263     0.418176621
    0.155158430     0.655158401     0.418175071
    0.998701811     0.999900639     0.449329376
    0.499900609     0.498701781     0.449329376
```

**6. penta-$SnS_2$**

```
    6.6360573769    0.0000000000    0.0000000000
    0.0000000000    6.6360573769    0.0000000000
    0.0000000000    0.0000000000   22.9979801178
  S   Sn
  4   2
Direct
    0.112559557     0.612559557     0.470771164
    0.887440443     0.387440443     0.470771164
    0.612559557     0.887440443     0.529228866
    0.387440443     0.112559557     0.529228866
    0.500000000     0.500000000     0.500000000
    0.000000000     0.000000000     0.500000000
```

**7. penta-$CdS_2$**

```
    5.4099440575    0.0000000000    0.0000000000
    0.0000000000    5.4099440575    0.0000000000
    0.0000000000    0.0000000000   28.0631027222
  S   Cd
  4   2
Direct
    0.137380779     0.637380779     0.447327435
    0.862619221     0.362619221     0.447327435
    0.637380779     0.862619221     0.552672565
    0.362619221     0.137380779     0.552672565
    0.500000000     0.500000000     0.500000000
    0.000000000     0.000000000     0.500000000
```

**8. penta-$SiC_2$**

```
    4.3971920013    0.0000000000    0.0000000000
    0.0000000000    4.3971920013    0.0000000000
    0.0000000000    0.0000000000   15.9183244705
  Si  C
   2  4
Direct
    0.999008298    0.999384344    0.449320823
    0.499384314    0.499008298    0.449320823
    0.608568728    0.889560521    0.491711318
    0.389560491    0.108568728    0.491711318
    0.890253305    0.390253276    0.406999320
    0.109224871    0.609224856    0.406936407
```