

VASPRUN SERVER TEST

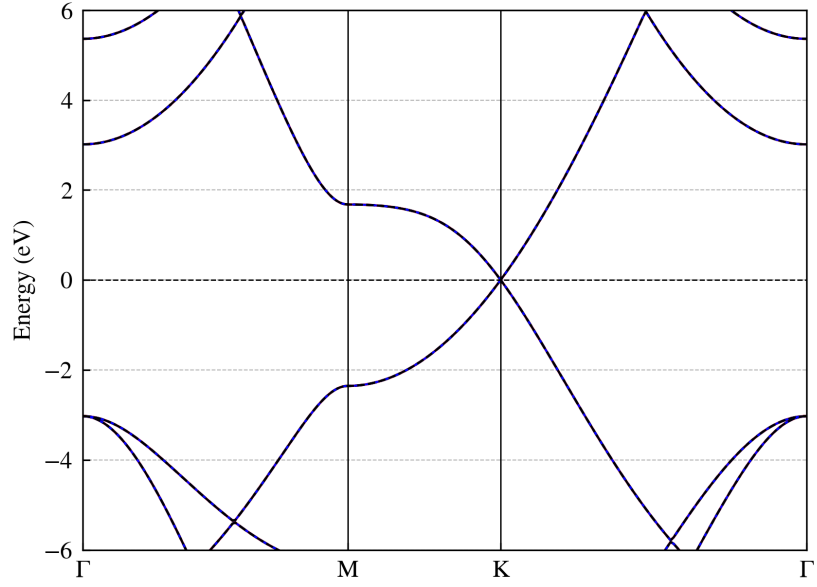
August 6, 2020

Contents

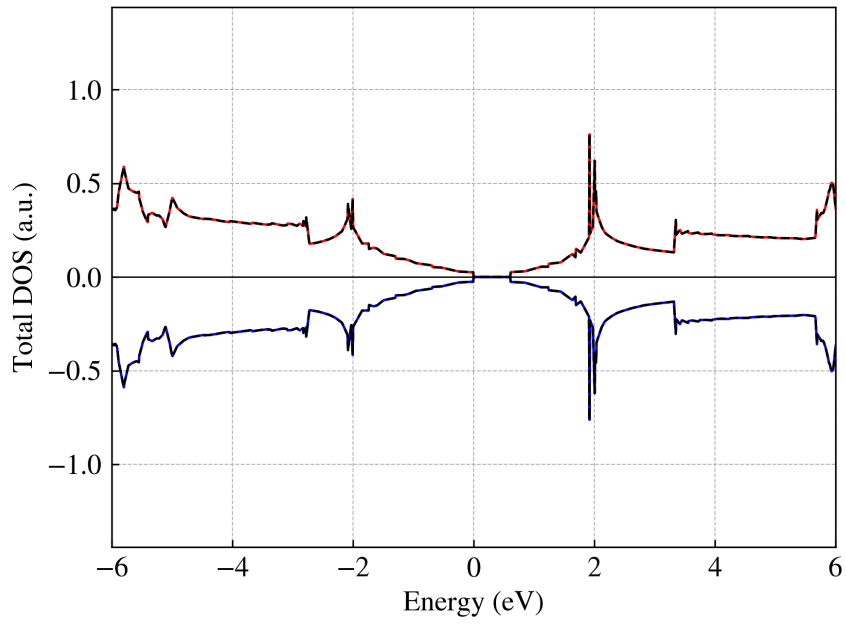
| | | |
|---|------------------------|---|
| 1 | [Object 1] Graphene-cl | 2 |
|---|------------------------|---|

1 [Object 1] Graphene-cl

| Items | | lib | calc. | diff. |
|----------------------|-------|---------------|---------------|--------------|
| CPUs | Nodes | 1 | 1 | 0 |
| | Cores | 20 | 20 | 0 |
| Time (s) | Relax | 158 | 156 | 2 |
| | SSC | 12 | 13 | -1 |
| | Band | 25 | 26 | -1 |
| | DOS | 6 | 6 | 0 |
| | Total | 201 | 201 | -1 |
| Lattice (Å) | a | 2.467309433 | 2.467309433 | 0.0 |
| | b | 2.467309433 | 2.467309433 | 0.0 |
| | c | 8.454534998 | 8.454534998 | 0.0 |
| Relaxed Force (eV/Å) | a | -0.000000e+00 | -0.000000e+00 | 0.000000e+00 |
| | b | 0.000000e+00 | 0.000000e+00 | 0.000000e+00 |
| | c | -0.000000e+00 | -0.000000e+00 | 0.000000e+00 |
| Fermi Energy (eV) | Relax | -0.7974 | -0.7974 | 0.0 |
| | SSC | -0.705 | -0.705 | 0.0 |
| | Band | -0.7038 | -0.7038 | 0.0 |
| | DOS | -1.0091 | -1.0091 | 0.0 |
| Total Energy (eV) | Relax | -18.46192516 | -18.46192516 | 0.0 |
| | SSC | -18.44900481 | -18.44900481 | 0.0 |
| | Band | -17.37228984 | -17.37228984 | 0.0 |
| | DOS | -18.44900159 | -18.44900159 | 0.0 |
| Band (eV) | Gap | 0.0465 | 0.0465 | 0.0 |
| | HOMO | 4 | 4 | 0 |
| | VBM | -0.0453 | -0.0453 | 0.0 |
| | Diff. | | 0.0 | |
| | Plot | See FIG.1(a) | | |
| DOS | Diff. | | 0.0 | |
| | Plot | See FIG.1(b) | | |
| Mag. (μ_B) | Relax | -0.0 | -0.0 | 0.0 |
| | SSC | -0.0 | -0.0 | 0.0 |
| | Band | -0.0 | -0.0 | 0.0 |
| | DOS | -0.0 | -0.0 | 0.0 |



(a) Band compare



(b) DOS compare

Figure 1: Band-DOS compare