Howto DFT+q

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vdW-DFq (van der Waals Density Functional Theory *q* form, or DFT+q) breaks the boundary of first-principles calculations by introducing one parameter q, leading to much higher accuracy. vdW-DFq method is also named "**DFT+q**", where the q value is an empirical parameter which is tunable to your system. Therefore, you might not be confused anymore on the selection of functionals for your system. The speed is good, only about 1.3 times standard PBE calculations. Please find the reference [S1] for details.

"Howto"use DFT+q method based on the VASP 5.4.4.

Step 0: please have the file **vdw_kernel.bindat** in the current working directory. This kernel file is available in VASP website (in potential files). You can also store this file somewhere (for example ~/vdw_kernal.bindat), then use it through a soft link (symbolic link) to save some disk space. Here is the command to create the soft link: "*ln -s ~/vdw_kernel.bindat vdw_kernel.bindat*"

Step 1: add the following to your INCAR file (the red 1.05 is the default q value) to activate this method.

```
GGA     = MK
LUSE_VDW = .TRUE.
PARAM1   = 0.1234
PARAM2   = 1.05
Zab_vdW  = -1.8867
AGGAC    = 0.0000
LASPH = .TRUE.
```

Step2: do geometry optimization (as your previous routine work) in vasp.

In general, q=1.05 will give a reasonably very good result. However, you can tune this q value to be better fit your required accuracy to the geometry parameters.

Step3 (optional): change the q value and redo the geometry optimization till your satisfactory.

Step4: using this q value for other quantities/parameters calculations.

[S1] Q. Peng, G. Wang, G.R.Liu, S.De, "van der Waals Density Functional Theory vdW-DFq for Semihard Materials", Crystals,(2019), **9**(5), 243. | [DOI: 10.3390/cryst9050243] | [online] | [local PDF] | [ResearchGate]*