Propriedades Quânticas de Nanomateriais utilizando a Teoria do Funcional Densidade (DFT)

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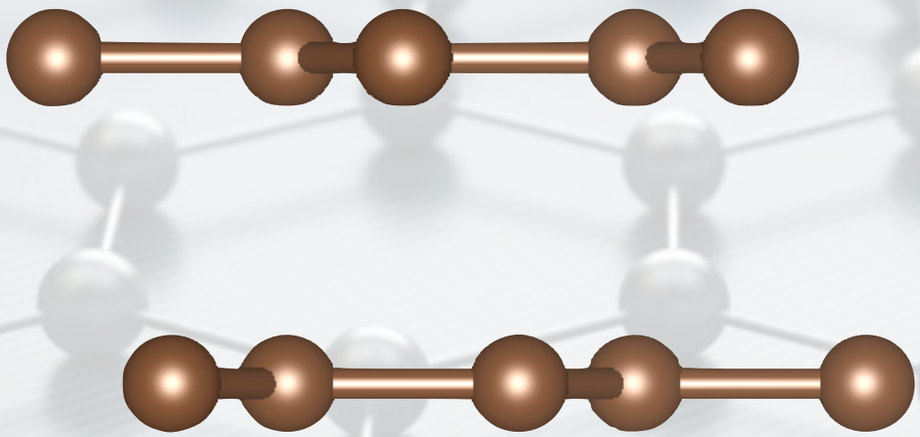
Outline

- Graphene bilayer with vdW corrections
- Output interpretation

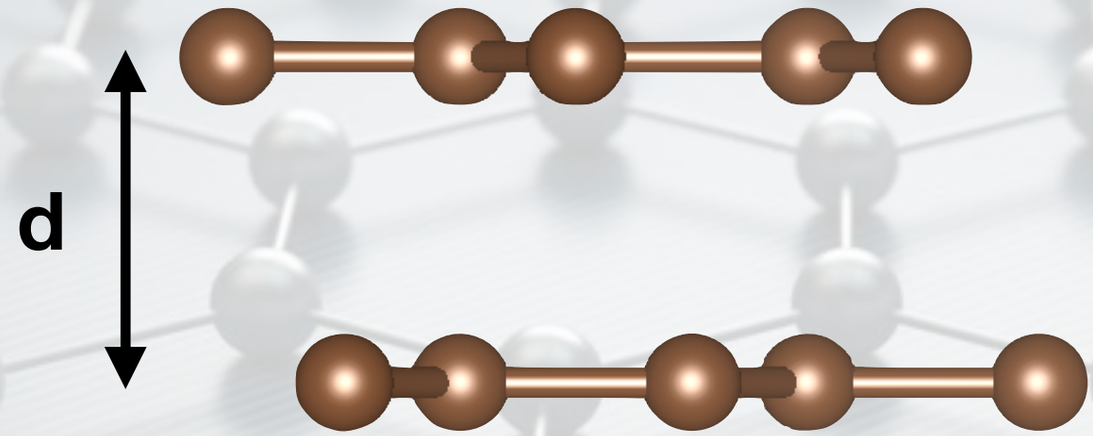
Graphene Bilayer

Interlayer distance



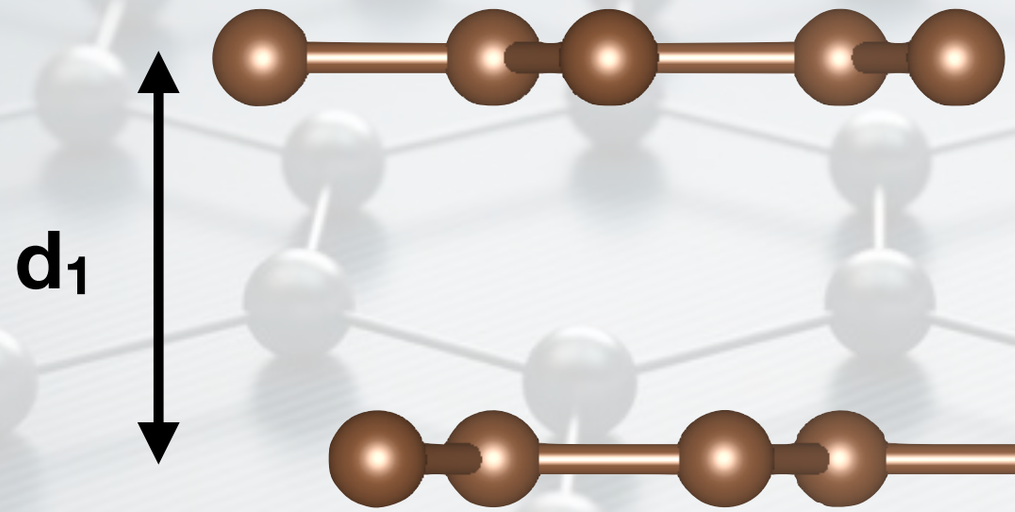
Graphene Bilayer

Interlayer distance



Graphene Bilayer

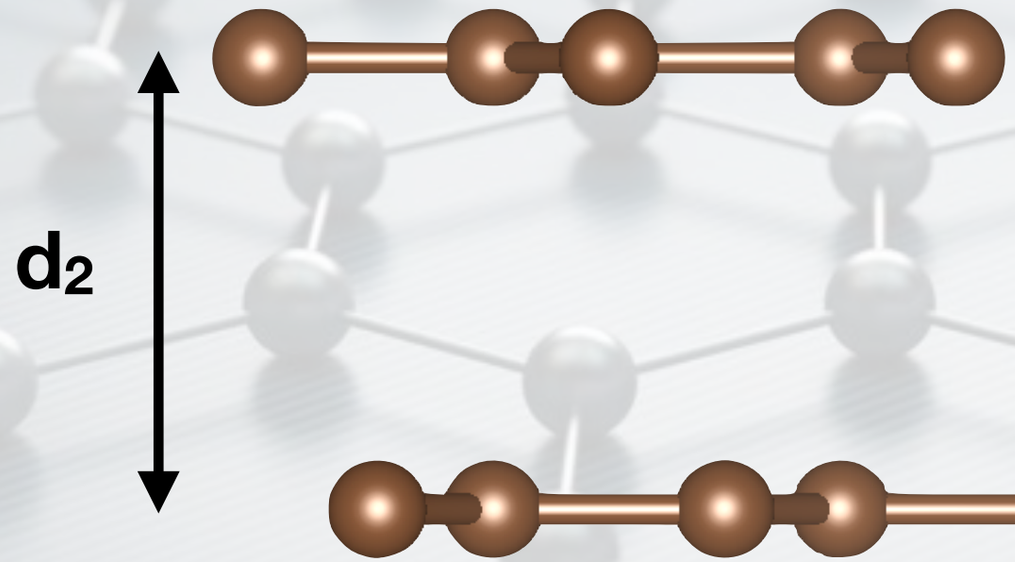
Interlayer distance



Total Energy

Graphene Bilayer

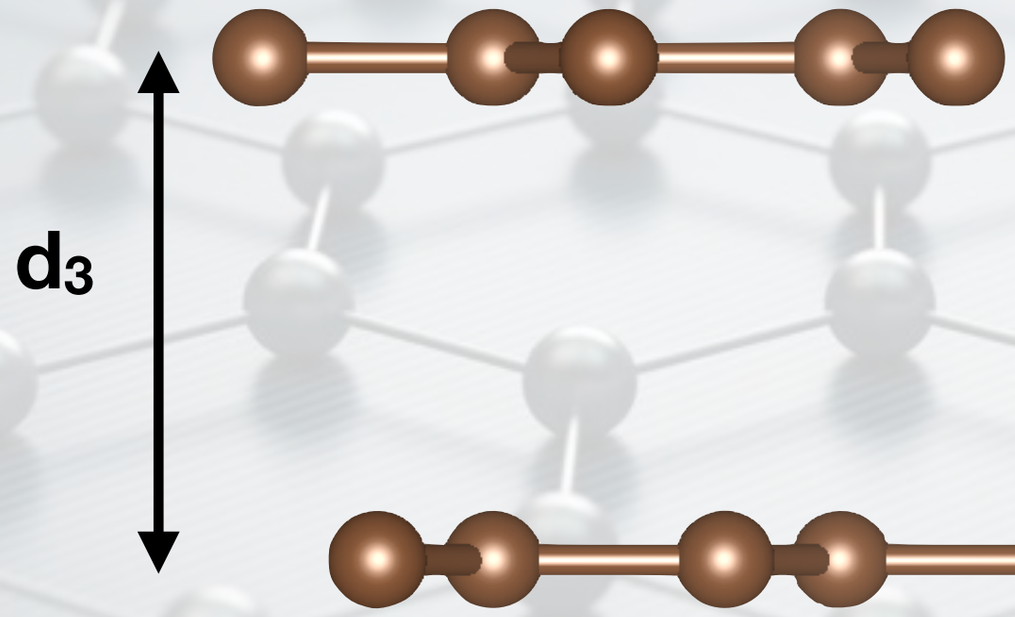
Interlayer distance



Total Energy

Graphene Bilayer

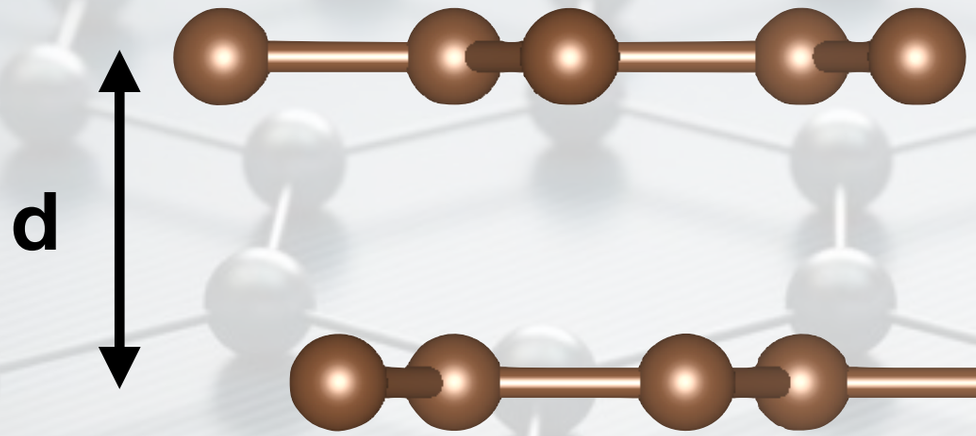
Interlayer distance



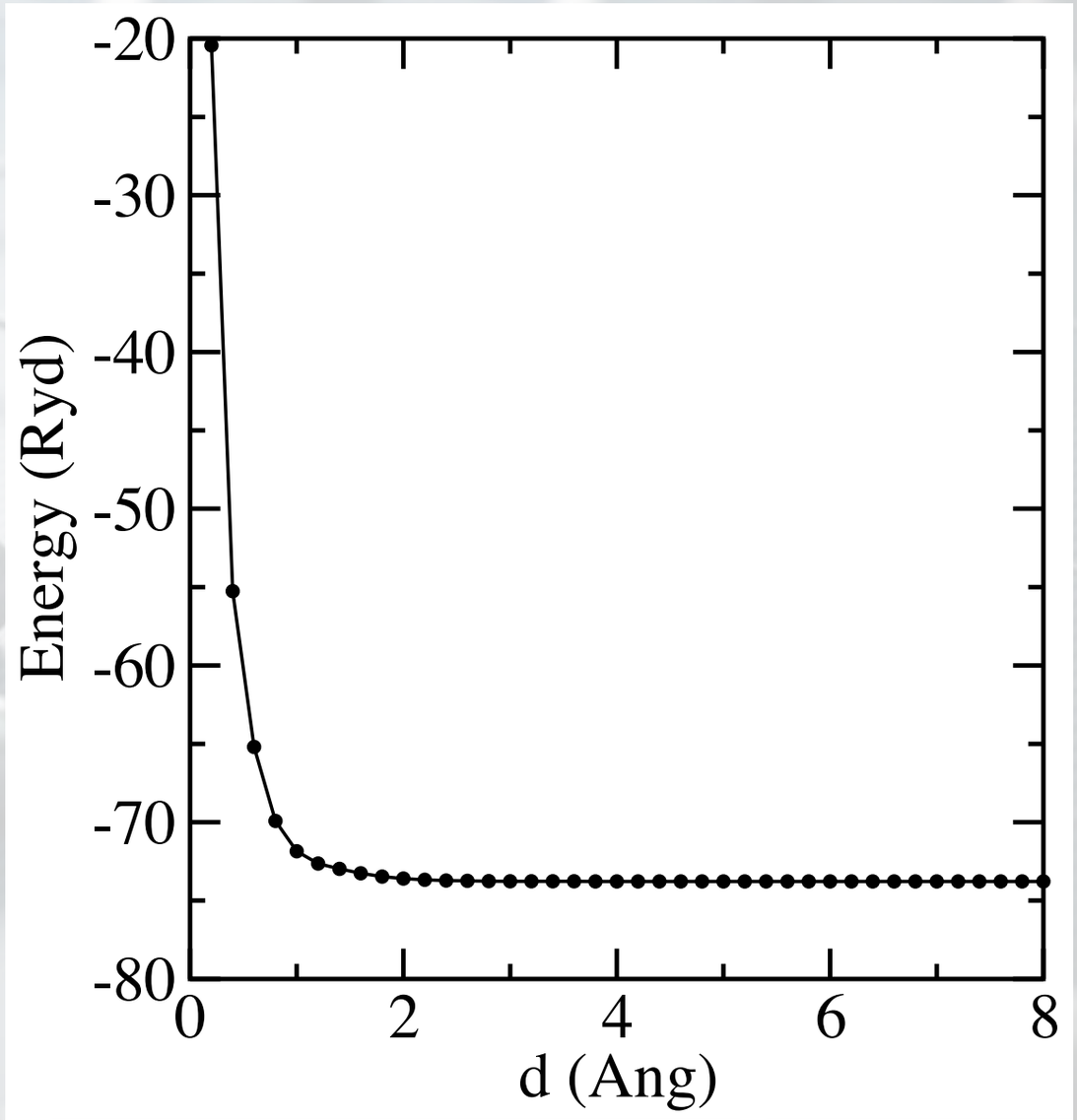
Total Energy

Graphene Bilayer

Interlayer distance

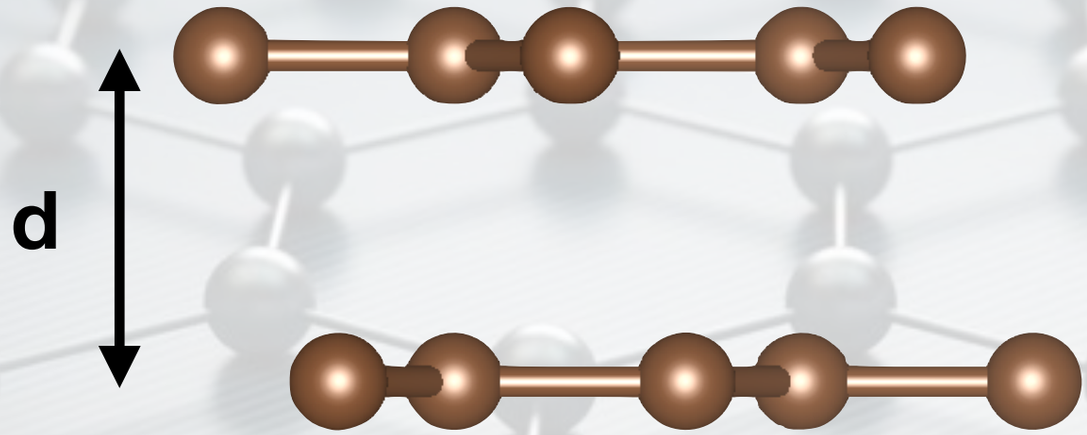


GGA

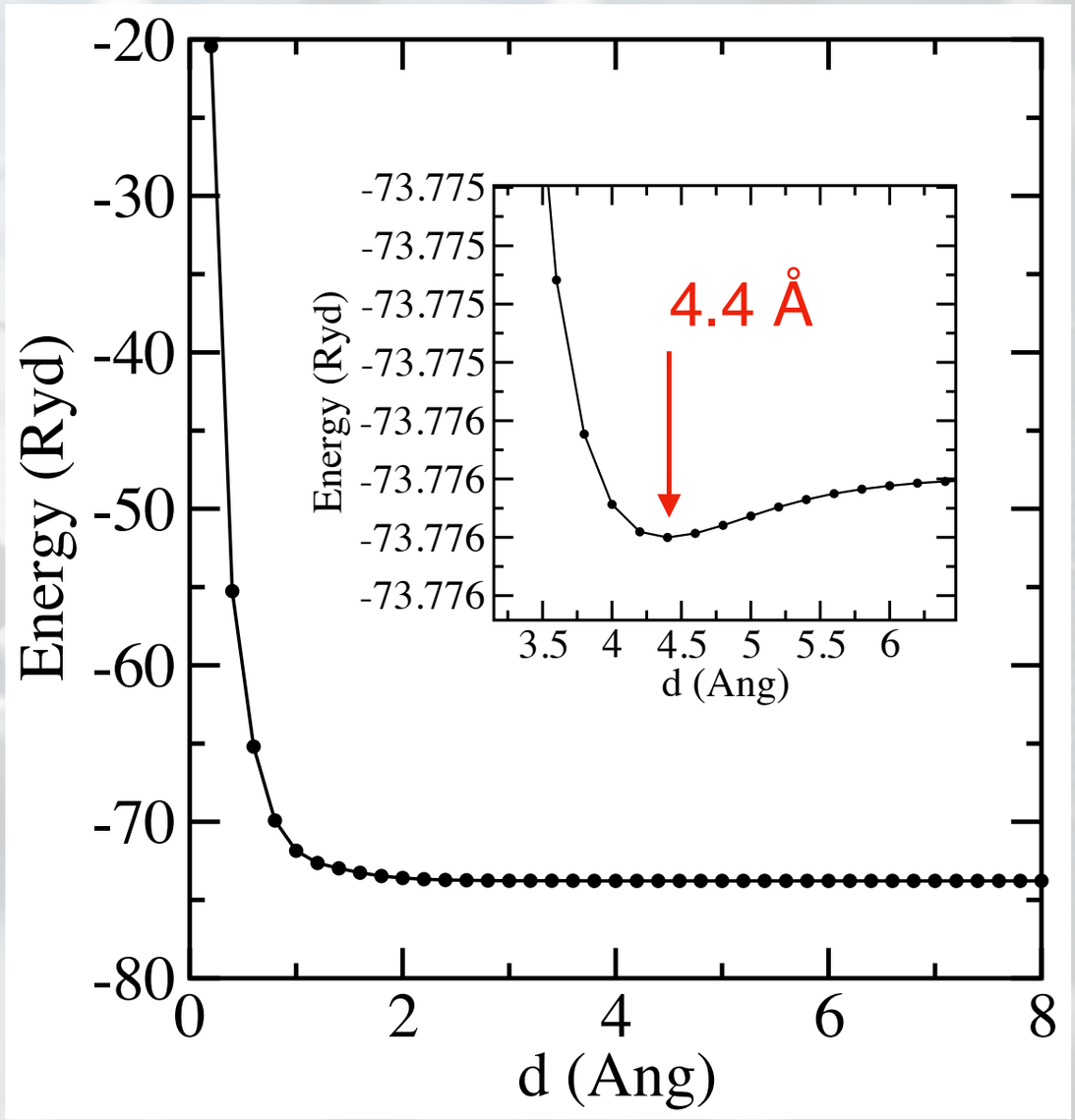


Graphene Bilayer

Interlayer distance

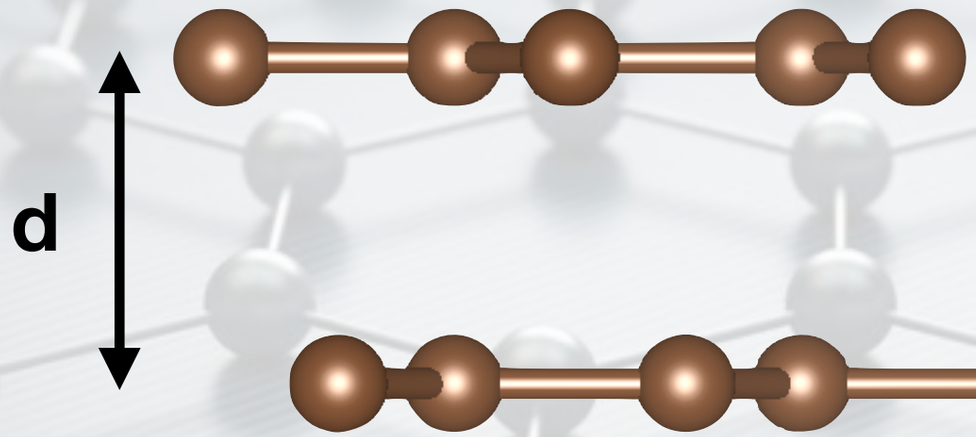


GGA

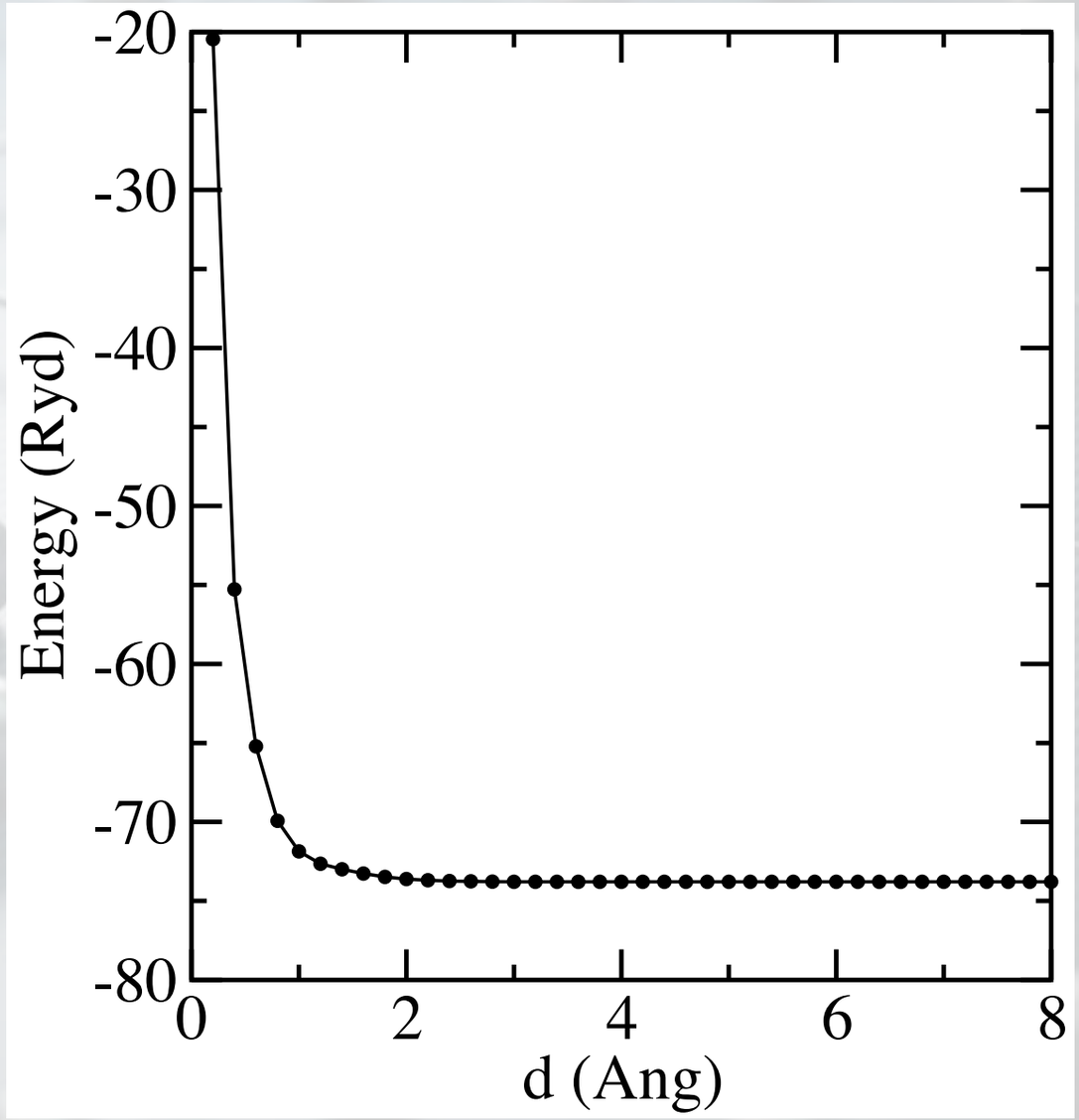


Graphene Bilayer

Interlayer distance

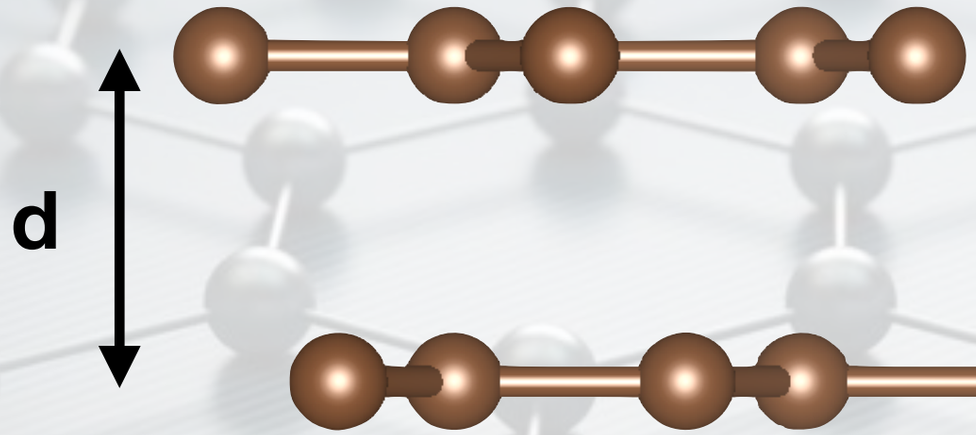


GGA+D3

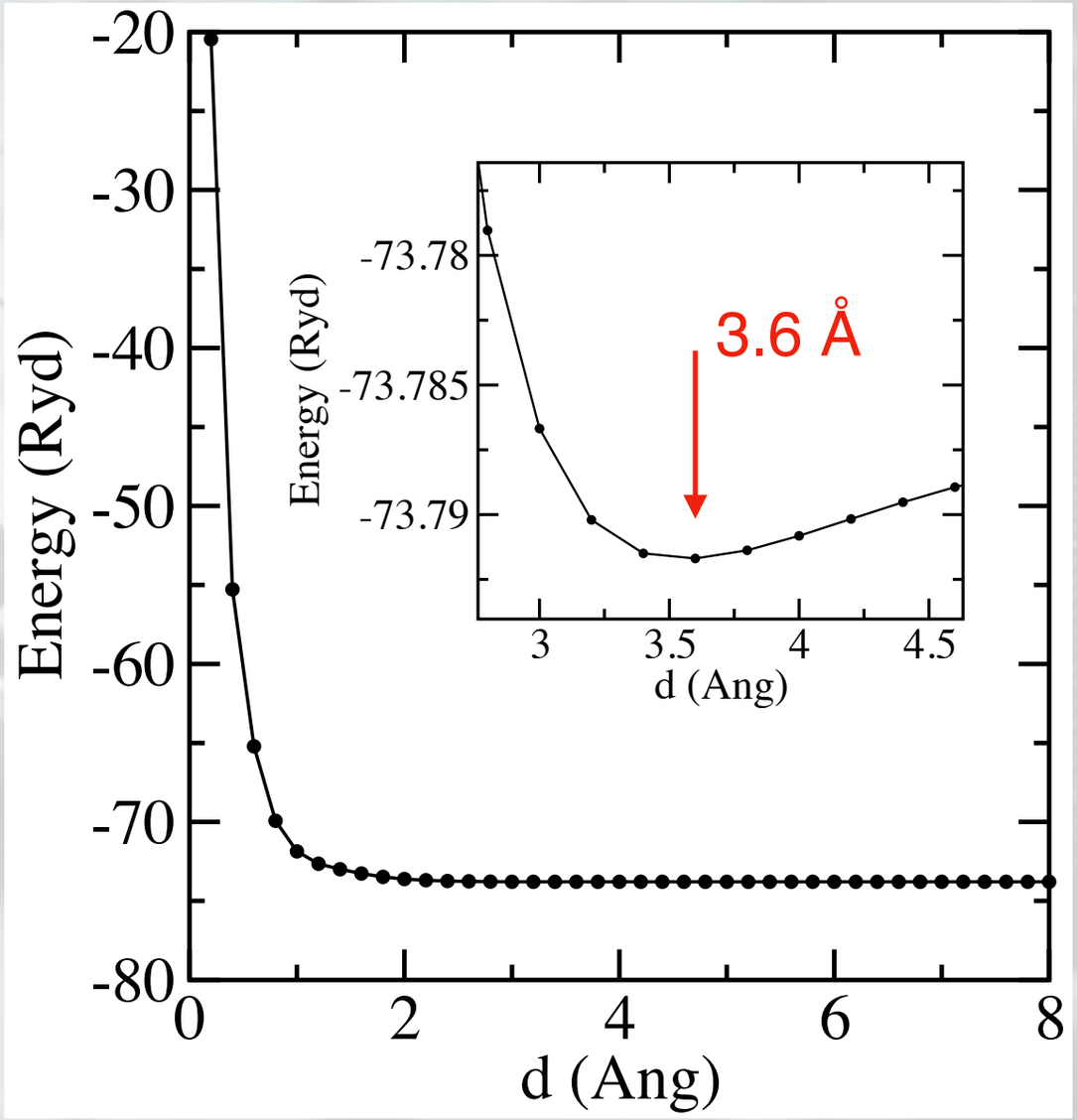


Graphene Bilayer

Interlayer distance



GGA+D3



Graphene Bilayer

```
&control
   calculation='scf',
   prefix='graphite'
   pseudo_dir = './',
   outdir='./'
 /
 &system
   ibrav = 4,
   a=2.46596482
   c=20.0
   nat=  4,
   ntyp= 1,
   vdw_corr = 'dft-d3',
   ecutwfc = 60
   ecutrho = 720
 /
 &electrons
   conv_thr =1.0d-8
/
ATOMIC_SPECIES
C 12.0107 C.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS crystal
 C 0.00000    1.00000    .65
 C 0.66667    0.33333    .65
 C 0.00000    1.00000    0.25000
 C 0.33333    0.66667    0.25000
K_POINTS AUTOMATIC
10 10 1 0 0 0
```

vdW corrections

Graphene Bilayer

&control

vdw_corr	CHARACTER
Default:	'none'
See:	london_s6, london_rcut, london_c6, london_rvdw, dftd3_version, dftd3_threebody, ts_vdw_econv_thr, ts_vdw_isolated, xdm_a1, xdm_a2

Type of Van der Waals correction. Allowed values:

'grimme-d2', 'Grimme-D2', 'DFT-D', 'dft-d' :
Semiempirical Grimme's DFT-D2. Optional variables:
london_s6, london_rcut, london_c6, london_rvdw
S. Grimme, J. Comp. Chem. 27, 1787 (2006), doi:10.1002/jcc.20495
V. Barone et al., J. Comp. Chem. 30, 934 (2009), doi:10.1002/jcc.21112

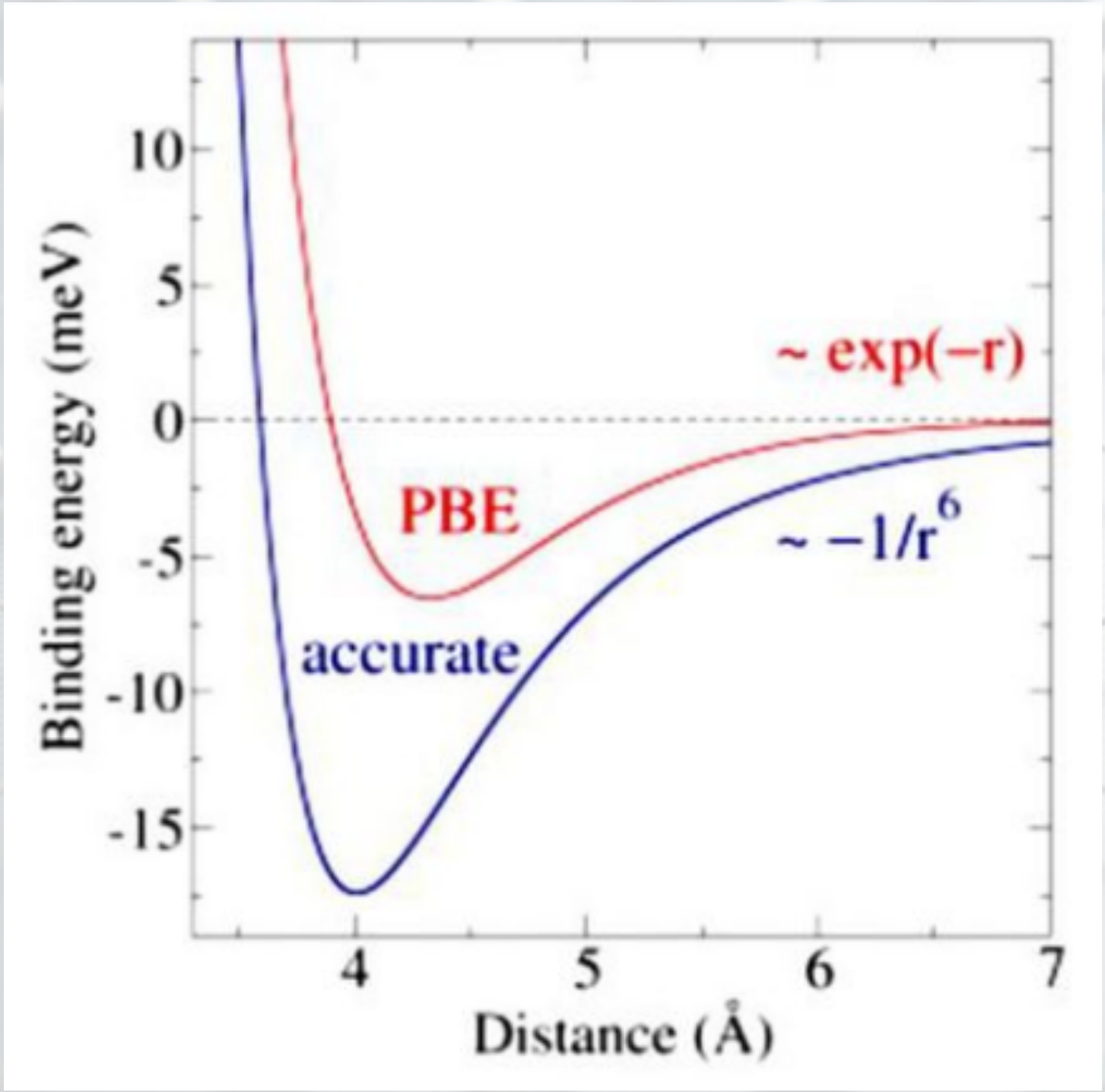
'grimme-d3', 'Grimme-D3', 'DFT-D3', 'dft-d3' :
Semiempirical Grimme's DFT-D3. Optional variables:
dftd3_version, dftd3_threebody
S. Grimme et al, J. Chem. Phys 132, 154104 (2010), doi:10.1002/jcc.20495

'TS', 'ts', 'ts-vdw', 'ts-vdW', 'tkatchenko-scheffler' :
Tkatchenko-Scheffler dispersion corrections with first-principle derived C6 coefficients.
Optional variables: ts_vdw_econv_thr, ts_vdw_isolated
See A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009).

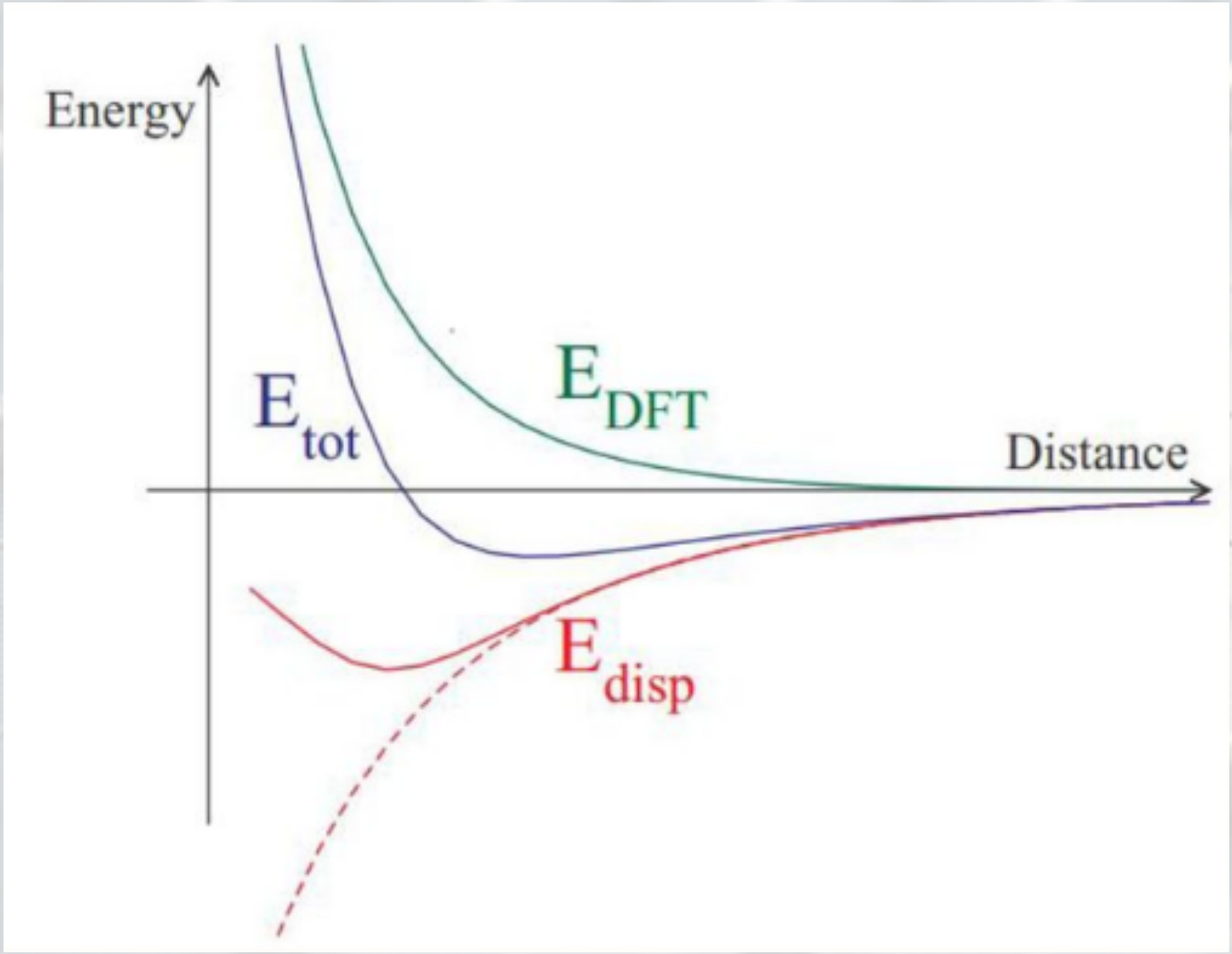
'XDM', 'xdm' :
Exchange-hole dipole-moment model. Optional variables: xdm_a1, xdm_a2
A. D. Becke et al., J. Chem. Phys. 127, 154108 (2007), doi:10.1063/1.2795701
A. Otero de la Roza et al., J. Chem. Phys. 136, 174109 (2012), doi:10.1063/1.4705760

Note that non-local functionals (eg vdw-DF) are NOT specified here but in input_dft

Graphene Bilayer

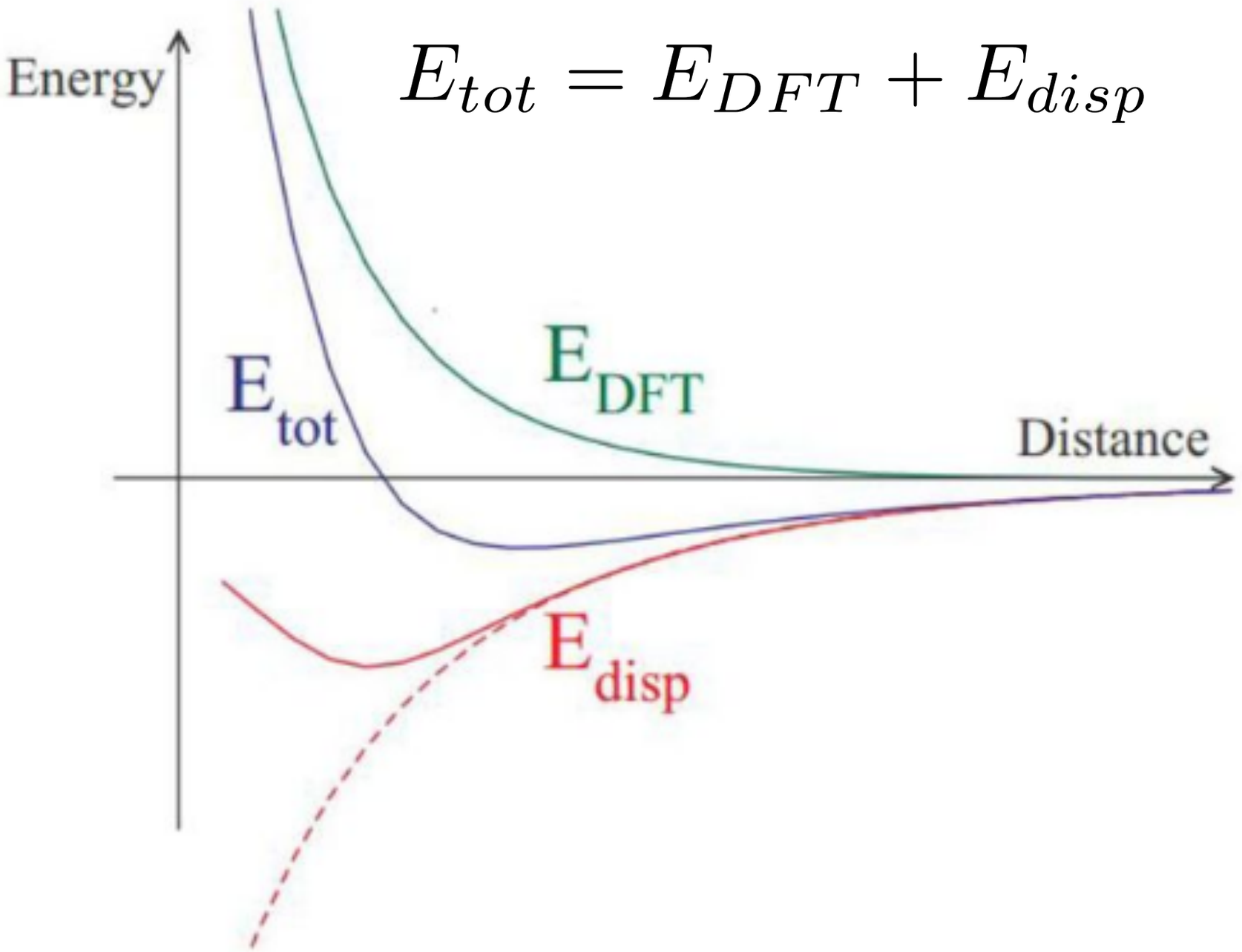


Graphene Bilayer



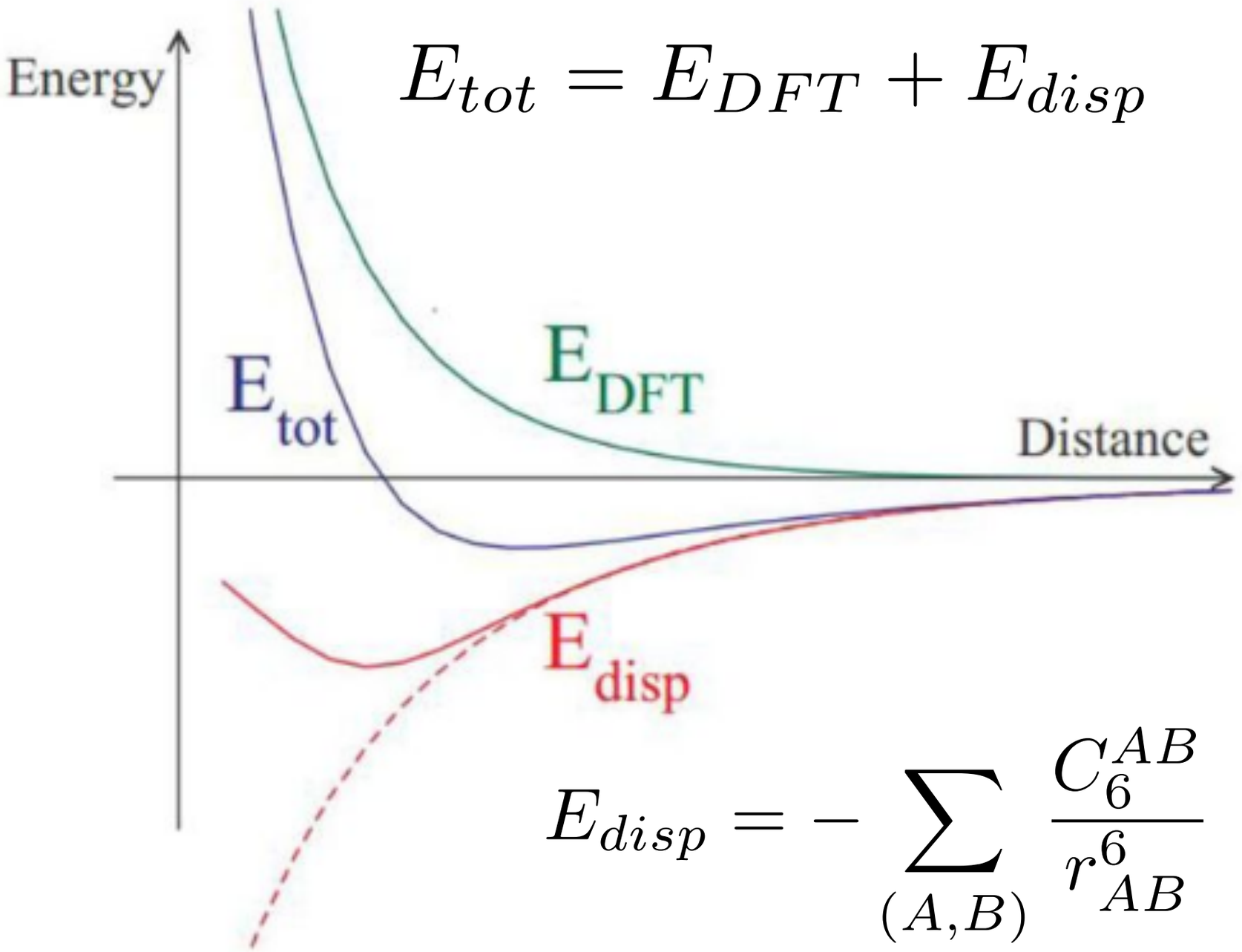
Graphene Bilayer

$$E_{tot} = E_{DFT} + E_{disp}$$



Graphene Bilayer

$$E_{tot} = E_{DFT} + E_{disp}$$



$$E_{disp} = -\sum_{(A,B)} \frac{C_6^{AB}}{r_{AB}^6}$$

Graphene Bilayer

&control

vdw_corr	CHARACTER
Default:	'none'
See:	london_s6, london_rcut, london_c6, london_rvdw, dftd3_version, dftd3_threebody, ts_vdw_econv_thr, ts_vdw_isolated, xdm_a1, xdm_a2

Type of Van der Waals correction. Allowed values:

'grimme-d2', 'Grimme-D2', 'DFT-D', 'dft-d' :
Semiempirical Grimme's DFT-D2. Optional variables:
london_s6, london_rcut, london_c6, london_rvdw
S. Grimme, J. Comp. Chem. 27, 1787 (2006), doi:10.1002/jcc.20495
V. Barone et al., J. Comp. Chem. 30, 934 (2009), doi:10.1002/jcc.21112

'grimme-d3', 'Grimme-D3', 'DFT-D3', 'dft-d3' :
Semiempirical Grimme's DFT-D3. Optional variables:
dftd3_version, dftd3_threebody
S. Grimme et al, J. Chem. Phys 132, 154104 (2010), doi:10.1002/jcc.20495

'TS', 'ts', 'ts-vdw', 'ts-vdW', 'tkatchenko-scheffler' :
Tkatchenko-Scheffler dispersion corrections with first-principle derived C6 coefficients.
Optional variables: ts_vdw_econv_thr, ts_vdw_isolated
See A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009).

'XDM', 'xdm' :
Exchange-hole dipole-moment model. Optional variables: xdm_a1, xdm_a2
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A. Otero de la Roza et al., J. Chem. Phys. 136, 174109 (2012), doi:10.1063/1.4705760

Note that non-local functionals (eg vdw-DF) are NOT specified here but in input_dft

Output

```
Program PWSCF v.6.5 starts on  4Jun2020 at 12:49:49

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
    "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
    "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
     URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Serial multi-threaded version, running on     1 processor cores
Waiting for input...
Reading input from standard input

Current dimensions of program PWSCF are:
Max number of different atomic species (ntypx) = 10
Max number of k-points (npk) =  40000
Max angular momentum in pseudopotentials (lmaxx) =  3
        file C.pbe-n-kjpaw_psl.1.0.0.UPF: wavefunction(s)  2S 2P renormalized

G-vector sticks info
--------------------
sticks:   dense  smooth     PW    G-vecs:    dense   smooth      PW
Sum         1069     361    109                115541    22353    3857
```

Output

Program PWSCF v.6.5 starts on 4Jun2020 at 12:49:49

**This program is part of the open-source Quantum ESPRESSO suite
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"P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
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URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote**

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G-vector sticks info
----

sticks:	dense	smooth	PW	G-vecs:	dense	smooth	PW
Sum	1069	361	109		115541	22353	3857

Output

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Program PWSCF v.6.5 starts on  4Jun2020 at 12:49:49

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Max angular momentum in pseudopotentials (lmaxx) =  3
        file C.pbe-n-kjpaw_psl.1.0.0.UPF: wavefunction(s)  2S 2P renormalized

G-vector sticks info
--------------------
sticks:   dense  smooth     PW    G-vecs:    dense   smooth      PW
Sum         1069     361    109                115541    22353    3857
```

Output

```
bravais-lattice index     =            4
lattice parameter (alat)  =       4.6531  a.u.
unit-cell volume          =     354.3310 (a.u.)^3
number of atoms/cell      =            2
number of atomic types    =            1
number of electrons       =         8.00
number of Kohn-Sham states=            8
kinetic-energy cutoff     =      60.0000  Ry
charge density cutoff     =     720.0000  Ry
convergence threshold     =      1.0E-08
mixing beta               =       0.7000
number of iterations used =            8  plain     mixing
Exchange-correlation= SLA PW PBX PBC
                    (   1   4   3   4   0   0   0)
```

Output

```
     celldm(1)=   4.653073  celldm(2)=   0.000000  celldm(3)=   4.061244
     celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

     crystal axes: (cart. coord. in units of alat)
               a(1) = (   1.000000   0.000000   0.000000 )
               a(2) = (  -0.500000   0.866025   0.000000 )
               a(3) = (   0.000000   0.000000   4.061244 )

     reciprocal axes: (cart. coord. in units 2 pi/alat)
               b(1) = (  1.000000  0.577350 -0.000000 )
               b(2) = (  0.000000  1.154701  0.000000 )
               b(3) = (  0.000000 -0.000000  0.246230 )
```

Output

```
atomic species   valence    mass     pseudopotential
   C              4.00    12.01070    C ( 1.00)

24 Sym. Ops., with inversion, found


                        s                frac. trans.

 isym =  1     identity

cryst.   s( 1) = (     1         0         0      )
                 (     0         1         0      )
                 (     0         0         1      )

cart.    s( 1) = (  1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


    isym =  2     180 deg rotation - cart. axis [0,0,1]

cryst.   s( 2) = (    -1         0         0      )
                 (     0        -1         0      )
                 (     0         0         1      )

cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000 -1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )
```

Output

```
atomic species   valence    mass     pseudopotential
   C              4.00    12.01070    C ( 1.00)

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                 (     0         1         0      )
                 (     0         0         1      )

cart.    s( 1) = (  1.0000000  0.0000000  0.0000000 )
                 (  0.0000000  1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )


   isym =  2     180 deg rotation - cart. axis [0,0,1]

cryst.   s( 2) = (    -1         0         0      )
                 (     0        -1         0      )
                 (     0         0         1      )

cart.    s( 2) = ( -1.0000000  0.0000000  0.0000000 )
                 (  0.0000000 -1.0000000  0.0000000 )
                 (  0.0000000  0.0000000  1.0000000 )
```

Output

point group D_6h(6/mmm)
there are 12 classes
the character table:

	E	2C6	2C3	C2	3C2'	3C2''	i	2S3	2S6	s_h	3s_d	3s_v
A_1g	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
A_2g	1.00	1.00	1.00	1.00	-1.00	-1.00	1.00	1.00	1.00	1.00	-1.00	-1.00
B_1g	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00
B_2g	1.00	-1.00	1.00	-1.00	-1.00	1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00
E_1g	2.00	1.00	-1.00	-2.00	0.00	0.00	2.00	1.00	-1.00	-2.00	0.00	0.00
E_2g	2.00	-1.00	-1.00	2.00	0.00	0.00	2.00	-1.00	-1.00	2.00	0.00	0.00
A_1u	1.00	1.00	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00
A_2u	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	1.00	1.00
B_1u	1.00	-1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00
B_2u	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	1.00	-1.00
E_1u	2.00	1.00	-1.00	-2.00	0.00	0.00	-2.00	-1.00	1.00	2.00	0.00	0.00
E_2u	2.00	-1.00	-1.00	2.00	0.00	0.00	-2.00	1.00	1.00	-2.00	0.00	0.00

Output

point group D_6h(6/mmm)
there are 12 classes
the character table:

	E	2C6	2C3	C2	3C2'	3C2''	i	2S3	2S6	s_h	3s_d	3s_v
A_1g	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
A_2g	1.00	1.00	1.00	1.00	-1.00	-1.00	1.00	1.00	1.00	1.00	-1.00	-1.00
B_1g	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00
B_2g	1.00	-1.00	1.00	-1.00	-1.00	1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00
E_1g	2.00	1.00	-1.00	-2.00	0.00	0.00	2.00	1.00	-1.00	-2.00	0.00	0.00
E_2g	2.00	-1.00	-1.00	2.00	0.00	0.00	2.00	-1.00	-1.00	2.00	0.00	0.00
A_1u	1.00	1.00	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00
A_2u	1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	1.00	1.00
B_1u	1.00	-1.00	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00
B_2u	1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	1.00	-1.00
E_1u	2.00	1.00	-1.00	-2.00	0.00	0.00	-2.00	-1.00	1.00	2.00	0.00	0.00
E_2u	2.00	-1.00	-1.00	2.00	0.00	0.00	-2.00	1.00	1.00	-2.00	0.00	0.00

Output

Cartesian axes

site n. atom positions (alat units)
1 C tau(1) = (0.0000000 0.5773503 2.0306218)
2 C tau(2) = (0.5000000 0.2886751 2.0306218)

Crystallographic axes

site n. atom positions (cryst. coord.)
1 C tau(1) = (0.3333333 0.6666667 0.5000000)
2 C tau(2) = (0.6666667 0.3333333 0.5000000)

number of k points= 19 Gaussian smearing, width (Ry)= 0.0200
cart. coord. in units 2pi/alat
k(1) = (0.0000000 0.0000000 0.0000000), wk = 0.0138889
k(2) = (0.0000000 0.0962250 0.0000000), wk = 0.0833333
k(3) = (0.0000000 0.1924501 0.0000000), wk = 0.0833333
k(4) = (0.0000000 0.2886751 0.0000000), wk = 0.0833333
k(5) = (0.0000000 0.3849002 0.0000000), wk = 0.0833333

Output

Cartesian axes

```
site n.     atom                  positions (alat units)
    1           C   tau(   1) = (   0.0000000   0.5773503   2.0306218  )
    2           C   tau(   2) = (   0.5000000   0.2886751   2.0306218  )
```

Crystallographic axes

```
site n.     atom                  positions (cryst. coord.)
    1           C   tau(   1) = (  0.3333333  0.6666667  0.5000000  )
    2           C   tau(   2) = (  0.6666667  0.3333333  0.5000000  )
```

```
number of k points=    19  Gaussian smearing, width (Ry)=  0.0200
                 cart. coord. in units 2pi/alat
  k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0138889
  k(    2) = (   0.0000000   0.0962250   0.0000000), wk =   0.0833333
  k(    3) = (   0.0000000   0.1924501   0.0000000), wk =   0.0833333
  k(    4) = (   0.0000000   0.2886751   0.0000000), wk =   0.0833333
  k(    5) = (   0.0000000   0.3849002   0.0000000), wk =   0.0833333
```

Output

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  k(    5) = (   0.0000000   0.3849002   0.0000000), wk =   0.0833333
```

Output

Self-consistent Calculation

```
iteration #  1     ecut=    60.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
   ethr =  1.00E-02,  avg # of iterations =  5.4

negative rho (up, down):  2.213E-06 0.000E+00

total cpu time spent up to now is        5.5 secs

   total energy              =     -36.85529971 Ry
Harris-Foulkes estimate   =     -36.97924302 Ry
 estimated scf accuracy    <       0.20269593 Ry

 iteration #  2     ecut=    60.00 Ry     beta= 0.70
     Davidson diagonalization with overlap
   ethr =  2.53E-03,  avg # of iterations =  3.5

negative rho (up, down):  5.731E-06 0.000E+00

total cpu time spent up to now is        7.6 secs

   total energy              =     -36.88692139 Ry
Harris-Foulkes estimate   =     -36.88717893 Ry
 estimated scf accuracy    <       0.00238499 Ry
```

Output

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```

Output

the Fermi energy is -0.4356 ev

! total energy = -36.88730505 Ry
Harris-Foulkes estimate = -36.88730505 Ry
estimated scf accuracy < 4.1E-10 Ry

total all-electron energy = -152.415500 Ry

The total energy is the sum of the following terms:

one-electron contribution = -90.46215956 Ry
hartree contribution = 47.22712924 Ry
xc contribution = -9.28079626 Ry
ewald contribution = 27.96304915 Ry
one-center paw contrib. = -12.33421418 Ry
-> PAW hartree energy AE = 19.00201147 Ry
-> PAW hartree energy PS = -18.98468017 Ry
-> PAW xc energy AE = -21.35347211 Ry
-> PAW xc energy PS = 9.00192663 Ry
-> total E_H with PAW = 47.24446054 Ry
-> total E_XC with PAW = -21.63234175 Ry
smearing contrib. (-TS) = -0.00031344 Ry

Output

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      -> PAW xc energy PS      =     9.00192663 Ry
      -> total E_H with PAW    =     47.24446054 Ry
      -> total E_XC with PAW   =    -21.63234175 Ry
     smearing contrib. (-TS)   =     -0.00031344 Ry
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Output

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```