k-point convergence for monolayer **5x5x1** (GGA, ENCUT = 500 eV, projected WF, bands_CRPA = 3*bands_SCF)

1x1x1

Final State

WF 1	4.60272578
WF 2	4.26111616

---

hopping parameters:

1	1	-0.735078
2	1	-1.329239
1	2	-1.329239
2	2	-2.979613

Eigenvalues:

-3.59699 no intersite
-0.11770 hoppings
dE = -3.4793

I	J	K	L	RE(V_IJKL)
1	1	1	1	6.9696557056
2	2	1	1	5.4432430445
2	1	2	1	0.2251331769
1	2	2	1	0.2251331769
2	1	1	2	0.2251331769
1	2	1	2	0.2251331769
1	1	2	2	5.4432430445
2	2	2	2	7.2543002885

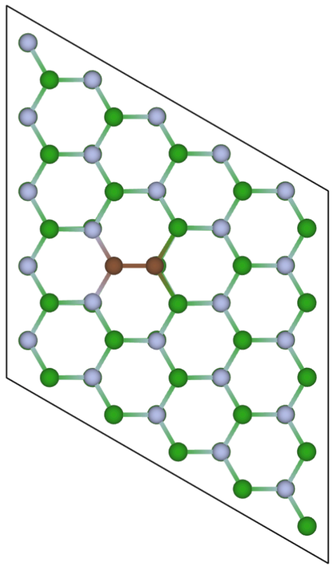
I	J	K	L	RE(W_IJKL)
1	1	1	1	3.8834473705
2	2	1	1	3.3224451994
2	1	2	1	0.1013326771
1	2	2	1	0.1013326771
2	1	1	2	0.1013326771
1	2	1	2	0.1013326771
1	1	2	2	3.3224451994
2	2	2	2	4.0270491752

Energy: 0.0;

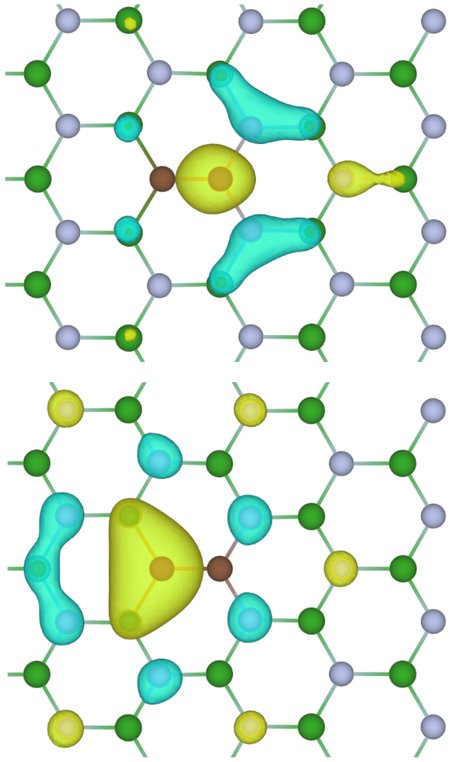
Energy: 2.846268 (3x);

Energy: 3.444549;

Energy: 6.765191



1x1x1

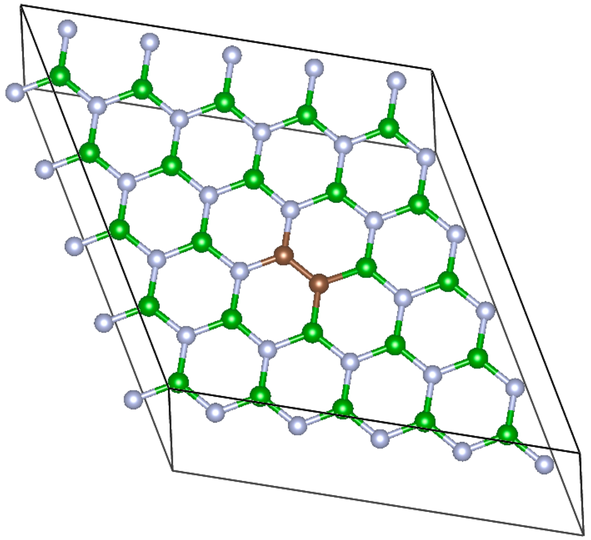


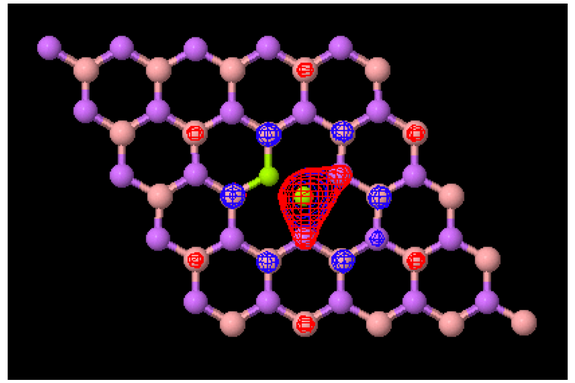
d(C-C) = 1.37(6,9) A

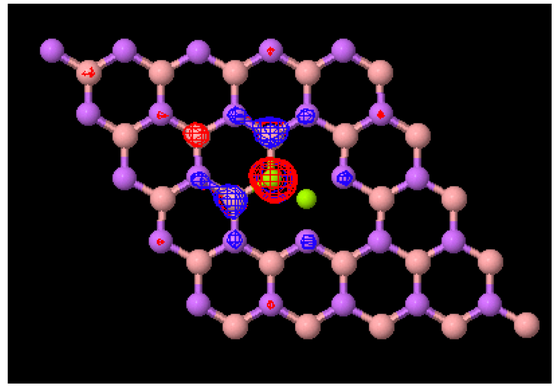
d(C-B) = 1.50(6,7) A

d(C-N) = 1.4(07,11) A

lo.PM







d(C-C) = 1.37809 A

d(C-B) = 1.50708 A

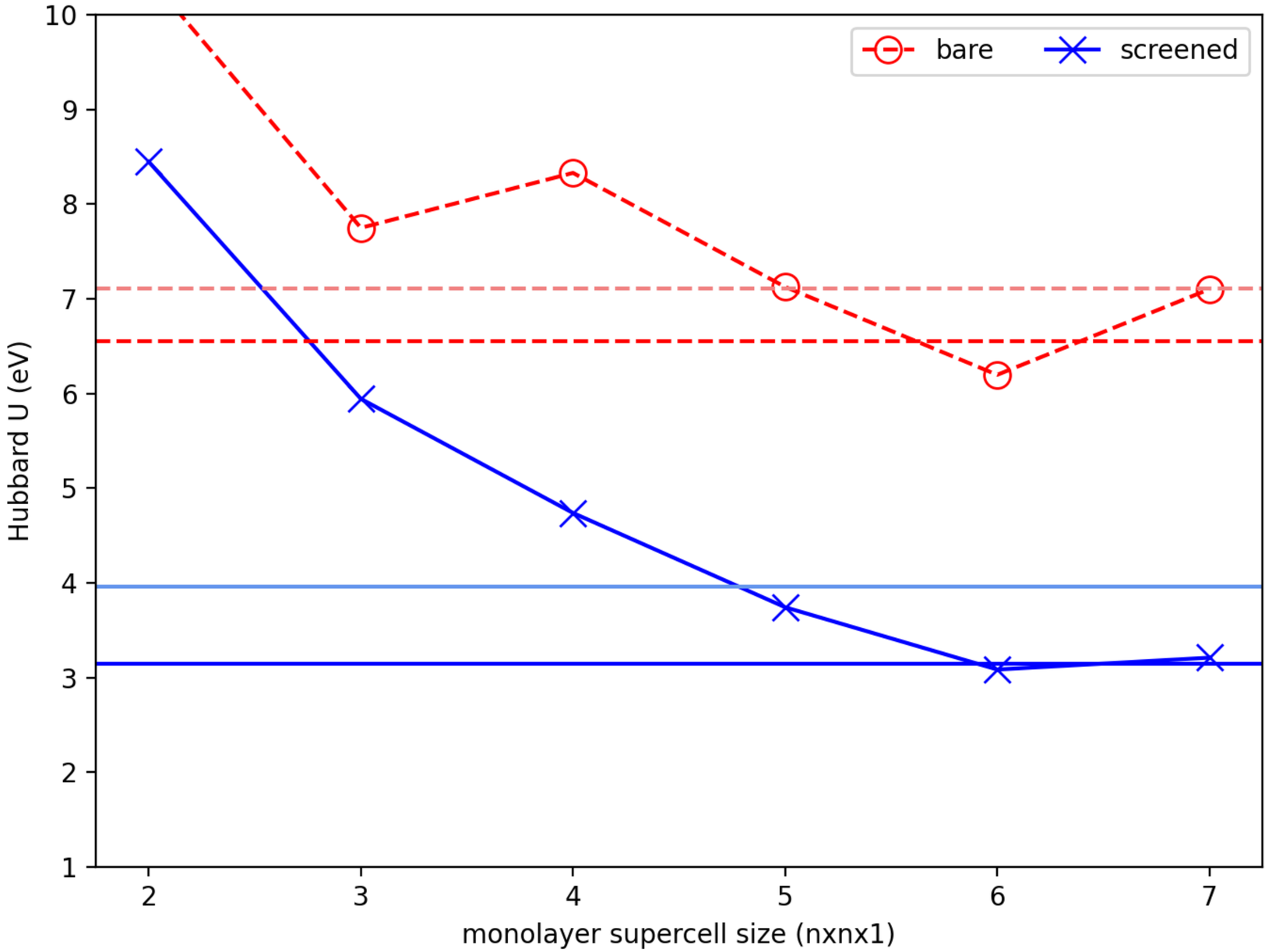
d(C-N) = 1.40981 A

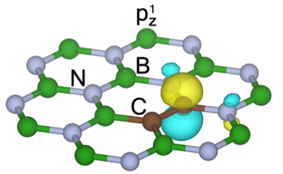
hopping, dE ok (**0.03, 0.05 eV diff.**)

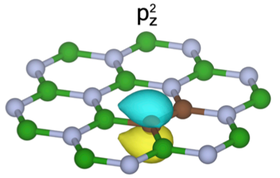
t =

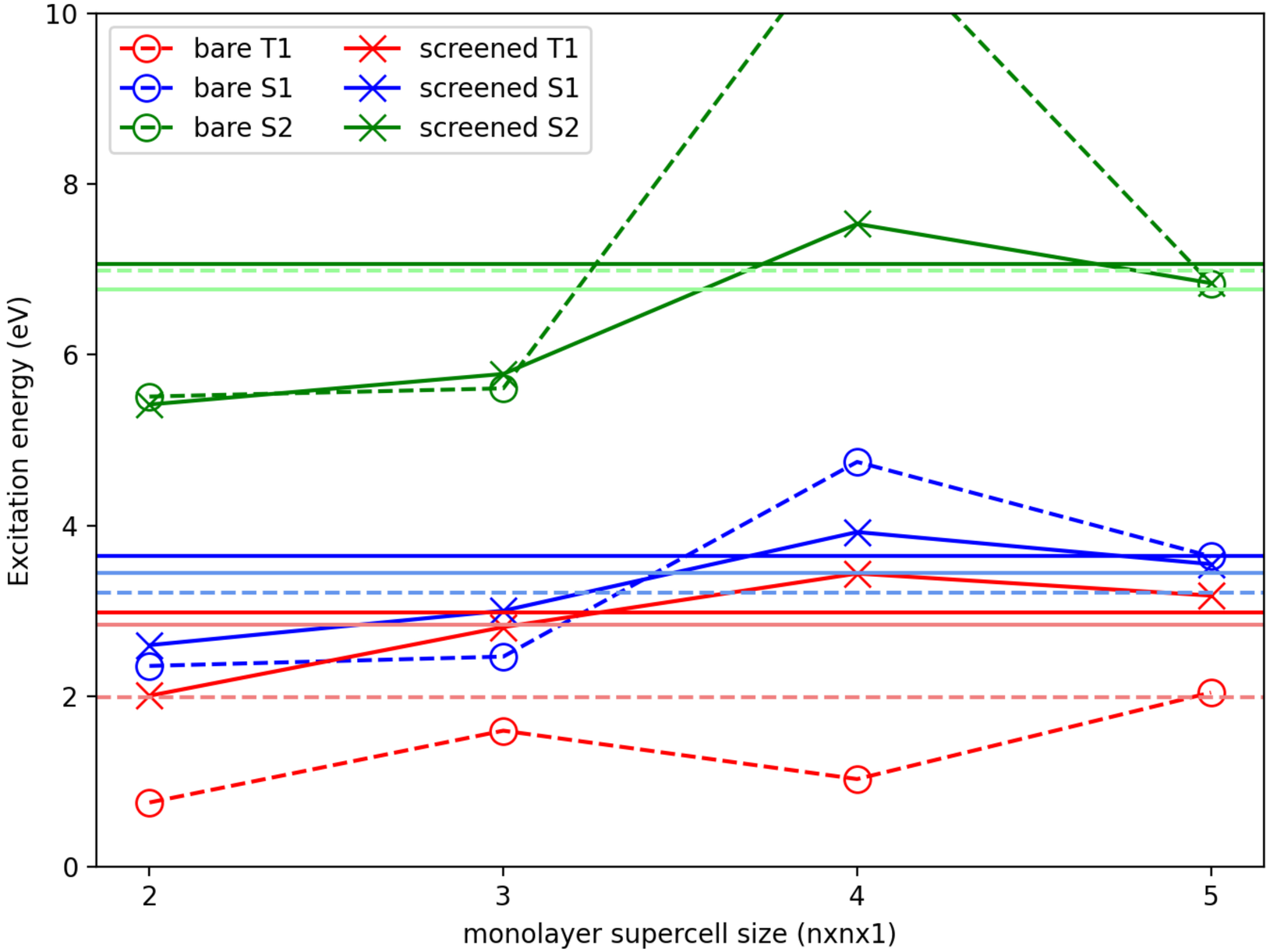
-2.51	-1.35
-1.35	-0.24

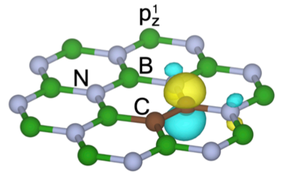
eigenvalues -3.139, 0.389 -> dE -3.527

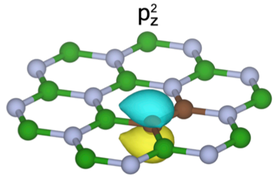

bare
screened
Hubbard U (eV)
monolayer supercell size (nxnx1)
10
9
8
7
6
5
4
3
2
1
2
3
4
5
6
7


p_z^1
B
N
C


p_z^2







Added Madelung constant to just (mm|mm),(mm|nn).

PM

5 Co 3d orbitals of NbCo

"For this construction we used per spin channel six states per Co atom, i.e., five 3d states and one 4s state"

PBE

average Coulomb integrals

Cluster	Bare (eV)	cRPA (eV)	RPA (eV)	ratio
literature	22.2	7.9	7.7	0.36
my data mix first 37 orbs def2-tzvpdd	22.91	8.77		0.38

```
Co 3d [33 32 31 34 35]
Co 4s [36]
```

Peters et al. PRB 2018

$$U(\omega) = [1 - vP_r(\omega)]v = \epsilon_r^{-1}v$$

$$\omega \to 0$$

$$U = \varepsilon^{-1}v \approx b^T(1-i)^{-1}b + Mb^T(1-i)^{-1}b/(b^Tb)$$

$$i_{PQ} = 2\sum_{ia} p_{ai}\frac{b_{Pai}b_{Qai}}{\varepsilon_i - \varepsilon_a}$$

density fitting basis: P,Q
canonical: a,i
localized: m,n

$$p_{ai} = 1 - \sum_n |U_{in}|^2 \sum_m |U_{am}|^2$$

= probability of transition

U is unitary matrix transforming
from canonical to active, localized orbitals