

A. Notations of cRPA UIJKL in VASP

In Silke's paper like PHYSICAL REVIEW B 86, 165105 (2012), the four-index partially screened interaction U_{ijkl}^{Silke} is defined as

$$U_{ijkl}^{\text{Silke}} = \lim_{\omega \rightarrow 0} \iint d\mathbf{r} d\mathbf{r}' w_i^*(\mathbf{r}) w_j^*(\mathbf{r}') \mathcal{U}(\mathbf{r}, \mathbf{r}', \omega) w_k(\mathbf{r}) w_l(\mathbf{r}'). \quad (1)$$

That is, the index order is chosen to yield a convenient order in the two-electron four orbital integrals.

However, in VASP U_{ijkl}^{VASP} is defined as

$$U_{ijkl}^{\text{VASP}} = \lim_{\omega \rightarrow 0} \iint d\mathbf{r} d\mathbf{r}' w_i^*(\mathbf{r}) w_k^*(\mathbf{r}') \mathcal{U}(\mathbf{r}, \mathbf{r}', \omega) w_j(\mathbf{r}) w_l(\mathbf{r}'). \quad (2)$$

This is the indices order that the files UIJKL and VIJKL generated from cRPA calculations use.

I J K L Re[UIJKL(VASP)] Im[UIJKL(VASP)]

Comparing Eq. (1) and Eq. (2), one could obtain

$$U_{ijkl}^{\text{Silke}} = U_{ikjl}^{\text{VASP}} \quad (3)$$

i.e., the intermediate two indices have exchanged.

Knowing this relationship, one could easily obtain the two index quantities

$$U_{mm'}^{\sigma, \bar{\sigma}} = U_{mm'mm'}^{\text{Silke}} = U_{mmmm'm'}^{\text{VASP}} \quad (4)$$

$$U_{mm'}^{\sigma, \sigma} = U_{mm'mm'}^{\text{Silke}} - U_{mm'm'm}^{\text{Silke}} = U_{mmmm'm'}^{\text{VASP}} - U_{mm'm'm}^{\text{VASP}} \quad (5)$$

In OUTCAR file from cRPA calculations, the reduced two-index quantities are given in terms of VASP notations. Take SrVO3 t2g for example.

screened Coulomb repulsion U_iiij between MLWFs:

	1	2	3
1	3.35797995	2.36462235	2.36462235
2	2.36462235	3.35797995	2.36462235
3	2.36462235	2.36462235	3.35797995

screened Coulomb repulsion U_ijji between MLWFs:

	1	2	3
1	3.35797995	0.45042559	0.45042559
2	0.45042559	3.35797995	0.45042559
3	0.45042559	0.45042559	3.35797995

So the first set U_iiij are interactions for antiparallel spins, i.e., U_{ijij}^{Silke} .

U_iiij - U_ijji(second set) are interactions for parallel spins, i.e., $U_{ijij}^{\text{Silke}} - U_{ijji}^{\text{Silke}}$.