

At date : processed

largest contribution to an MCI for each group
 Significant secondary contribution to an MCI

Element	MCI1	MCI2	MCI3	MCI4	MCI5	MCI6	MCI7	MCI8	MCI9	MCI10	MCI11	MCI12	MCI13	MCI14	MCI15
I group															
I	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pe	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pz	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
II group															
I	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pe	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pz	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
III group															
I	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pe	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Py	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pz	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

A bonding-antibonding pair of MCIs

Element	MCI1	MCI2
I group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00
II group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00
III group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00

MCI1 is bonding - all contributions have the same sign

MCI2 is antibonding - the I contribution has the opposite sign to the II contributions

A pair of mixing MCIs

Element	MCI1	MCI2
I group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00
II group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00
III group		
I	0.00	0.00
Pe	0.00	0.00
Py	0.00	0.00
Pz	0.00	0.00

We can see that the secondary contributions (yellow) in MCI1 line up exactly with the primary contributions (green) in MCI2 and vice versa. This shows us that mixing is occurring