

Bond analysis SHE AuRn+

E-mail:

Results

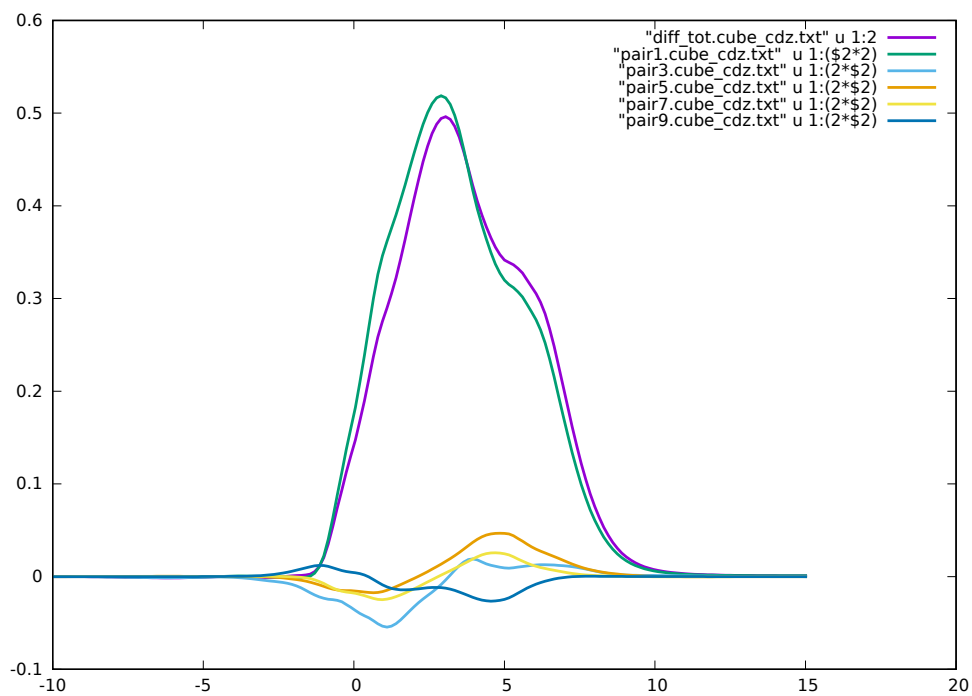
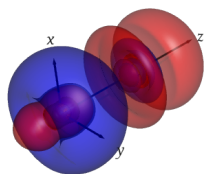
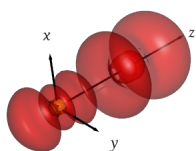


Figure 1

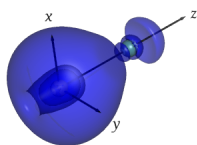
DEint	-47.4012
DEtildePauli	85.5963
DEexc	-24.0878
DEpauli	61.5084
DEelect	-45.6129
DEorb	-63.2968
nocv1	-0.1193



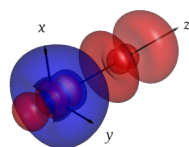
$$\Delta\rho'$$



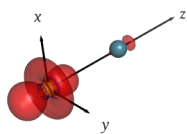
$$|\varphi_{-1}|^2$$



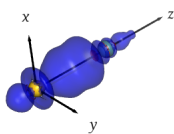
$$|\varphi_{+1}|^2$$



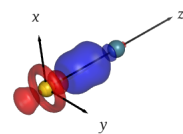
$$\Delta\rho'_1$$



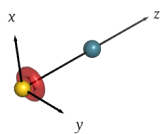
$$|\varphi_{-2}|^2$$



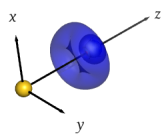
$$|\varphi_{+2}|^2$$



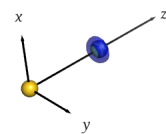
$$\Delta\rho'_2$$



$$|\varphi_{-3}|^2$$



$$2|\varphi_{+3}|^2$$



$$\Delta\rho'_3$$

CT nocv1	0.490026
CT nocv2	-0.023532
CT nocv3	0.003218
CT nocv4	-0.007912
CT nocv5	-0.012522
CT nocv6	-0.003216
CT tot	0.450352
CT tot ortho	0.442308