Bond analysis SHE AuFl+

E-mail:

Results
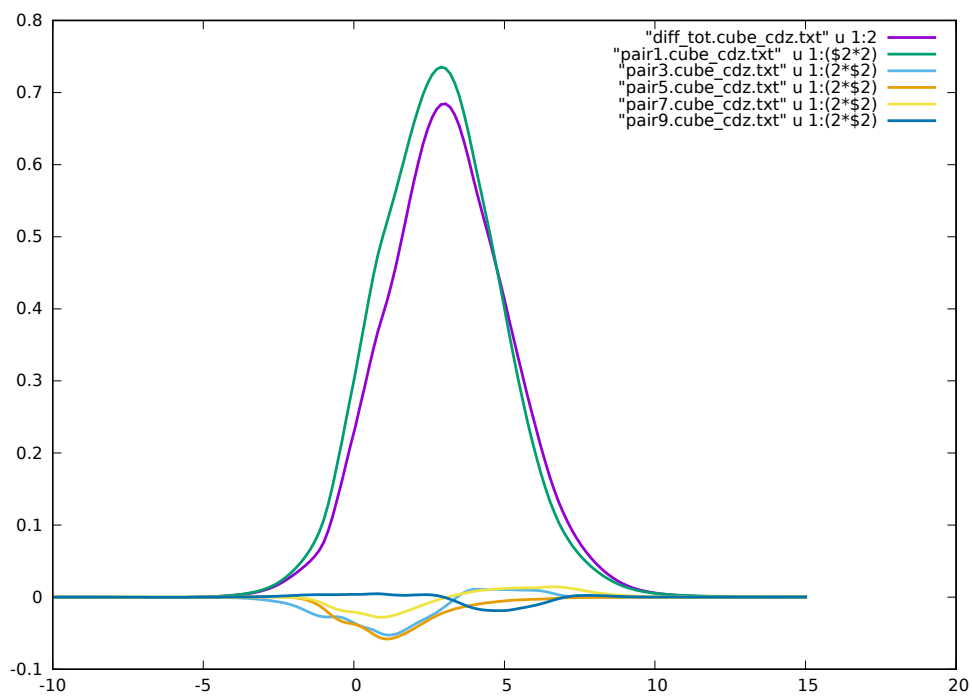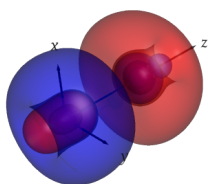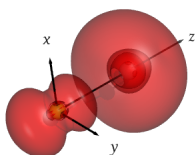

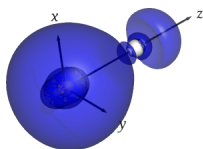Figure 1

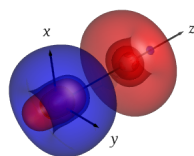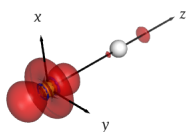|	
DEint	-65.6807
DEtildePauli	72.1223
DEexc	-19.9776
DEpauli	52.1447
DEelect	-39.1422
DEorb	-78.6832
nocv1	-0.0552

$\Delta\rho'$

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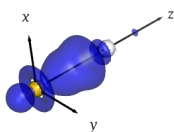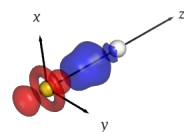
$|\varphi_{+1}|^2$

$\Delta\rho'_1$

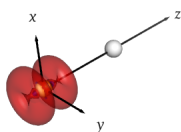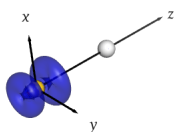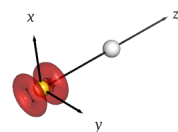$|\varphi_{-2}|^2$

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

$\Delta\rho'_2$

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

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

$\Delta\rho'_3$

CT nocv1	0.714536
CT nocv2	-0.027708
CT nocv3	-0.031918
CT nocv4	-0.008188
CT nocv5	0.0034
CT nocv6	-0.002654
CT tot	0.651476
CT tot ortho	0.648890