Bond analysis SHE AuHg+

E-mail:

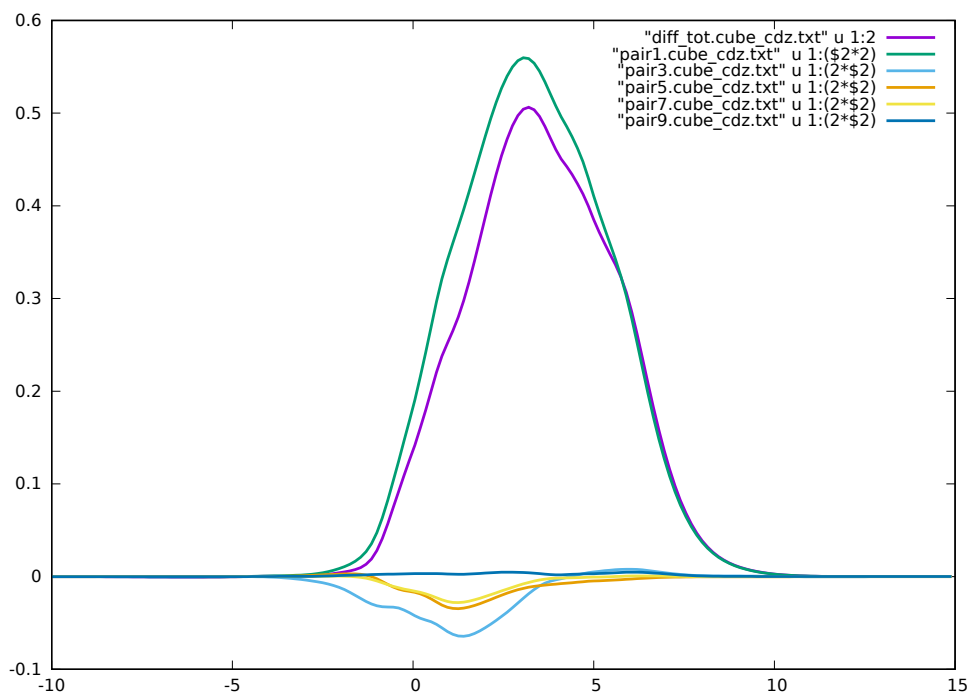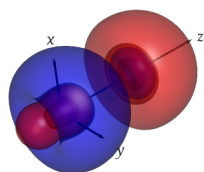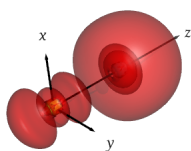## Results

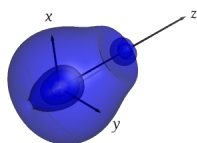
Figure 1

DEint	-51.1341
DEtildePauli	80.4823
DEexc	-25.9427
DEpauli	54.5396
DEelect	-42.5393
DEorb	-63.1344
nocv1	-0.4682

$\Delta\rho'$

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

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

$\Delta\rho'_1$

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

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

$\Delta\rho'_2$
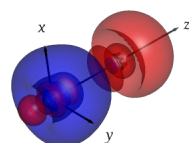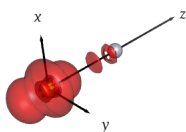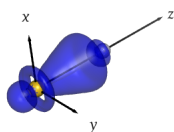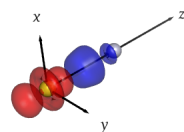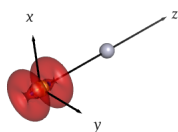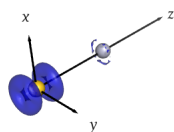
$\left|\varphi_{-3}\right|^2$

$\left|\varphi_{+3}\right|^2$
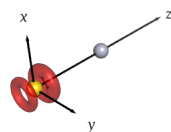
$\Delta\rho'_3$

CT nocv1	0.477012
CT nocv2	0.000208
CT nocv3	-0.006694
CT nocv4	-0.001326
CT nocv5	0.002366
CT nocv6	-0.001138
CT tot	0.435710
CT tot ortho	0.461715