Bond analysis SHE AuOg+

E-mail:

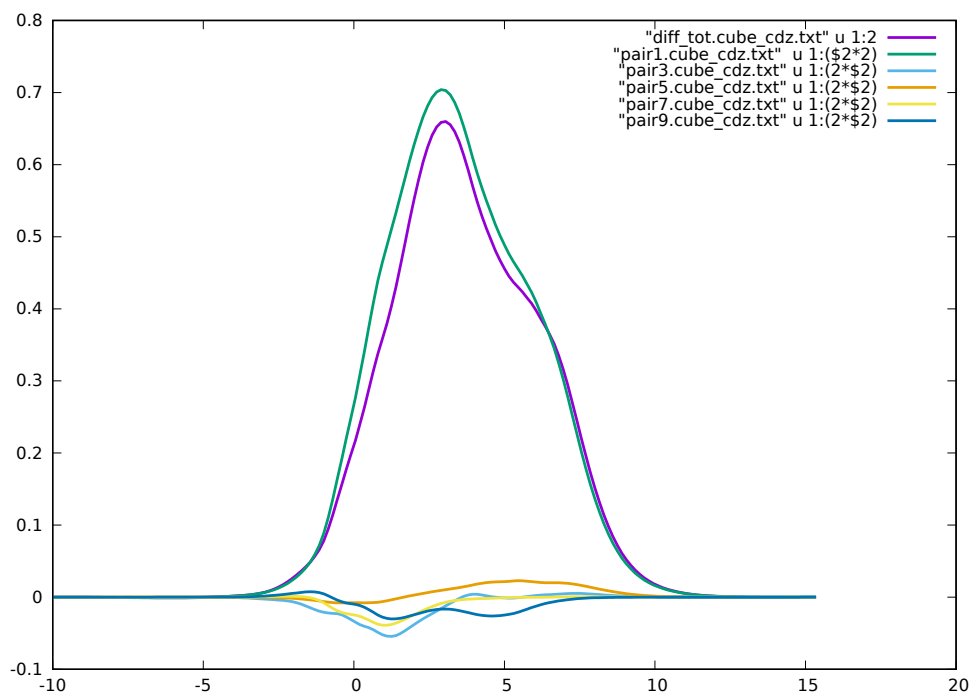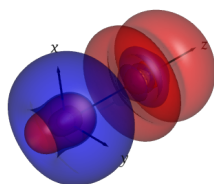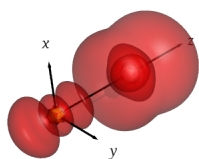## Results

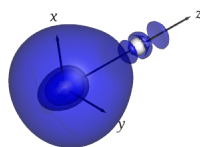
Figure 1

DEint	-69.6545
DEtildePauli	81.6895
DEexc	-23.3315
DEpauli	58.3580
DEelect	-46.2992
DEorb	-81.7133
nocv1	-0.1734

$$\Delta\rho'$$
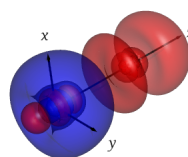
$$|\varphi_{-1}|^2 \qquad\qquad |\varphi_{+1}|^2 \qquad\qquad \Delta\rho'_1$$
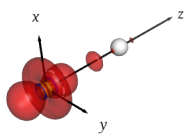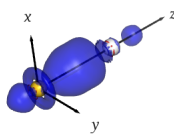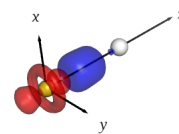
$$|\varphi_{-2}|^2 \qquad\qquad |\varphi_{+2}|^2 \qquad\qquad \Delta\rho'_2$$
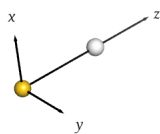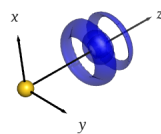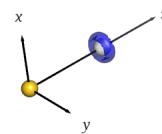
$$|\varphi_{-3}|^2 \qquad\qquad \overset{2}{|\varphi_{+3}|^2} \qquad\qquad \Delta\rho'_3$$

CT nocv1	0.68691
CT nocv2	-0.024638
CT nocv3	0.00691
CT nocv4	-0.014378
CT nocv5	-0.018664
CT nocv6	-0.002708
CT tot	0.632027
CT tot ortho	0.633309