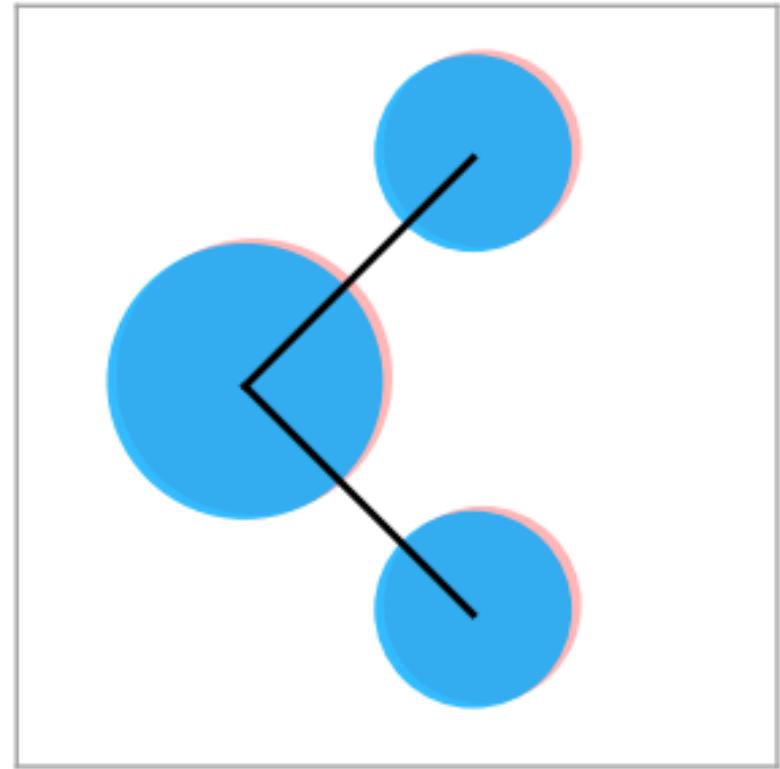
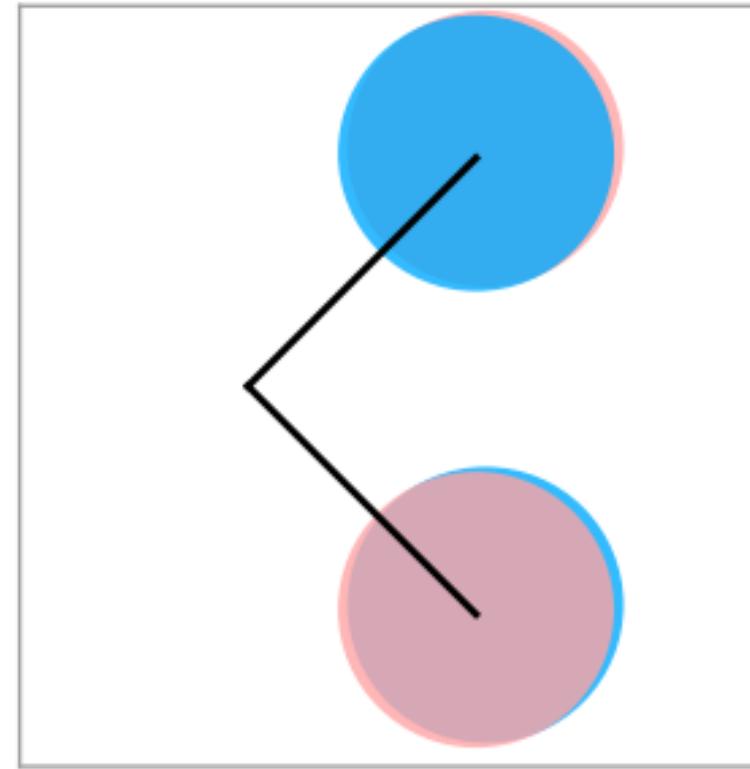


MO 1
2e



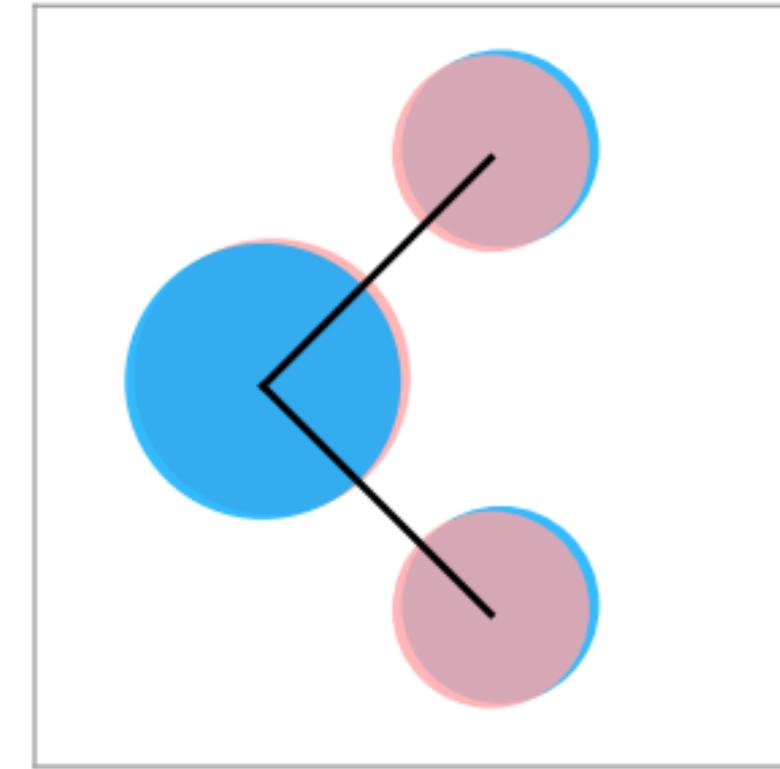
$\alpha + 1.41\beta$

MO 2
2e



α

MO 3
0e



$\alpha - 1.41\beta$

$\alpha - 1.5 \beta$



$\alpha - 1.0 \beta$



$\alpha - 0.5 \beta$



α

$\alpha + 0.5 \beta$



$\alpha + 1.0 \beta$



$\alpha + 1.5 \beta$



E: $4\alpha + 2.83\beta$
E_atom/N: $0.94|\beta|$
gap: $1.41|\beta|$
 η : $0.71|\beta|$

σ skeleton

Bond orders and atomic charges

