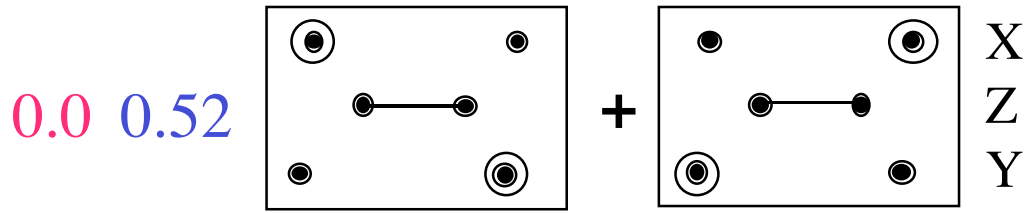


MO Theory
Pretty obvious

The Problem

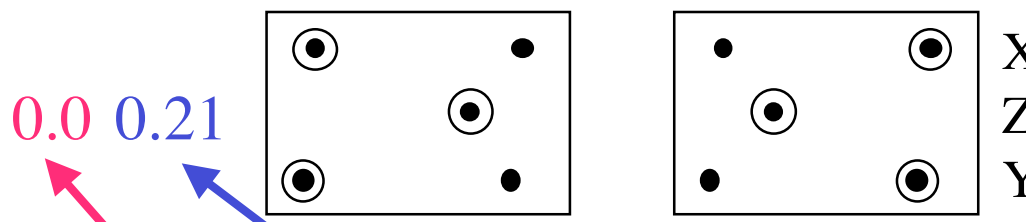
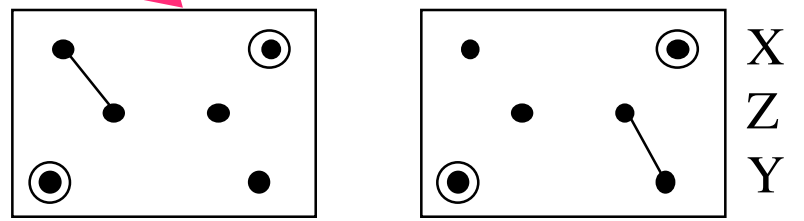
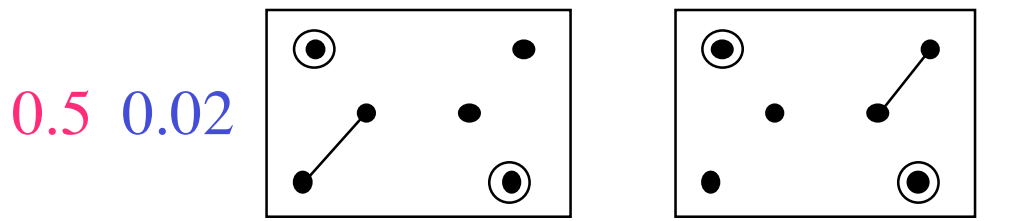


Carsten Byrman
1995
EZPP basis



molecule

atomic

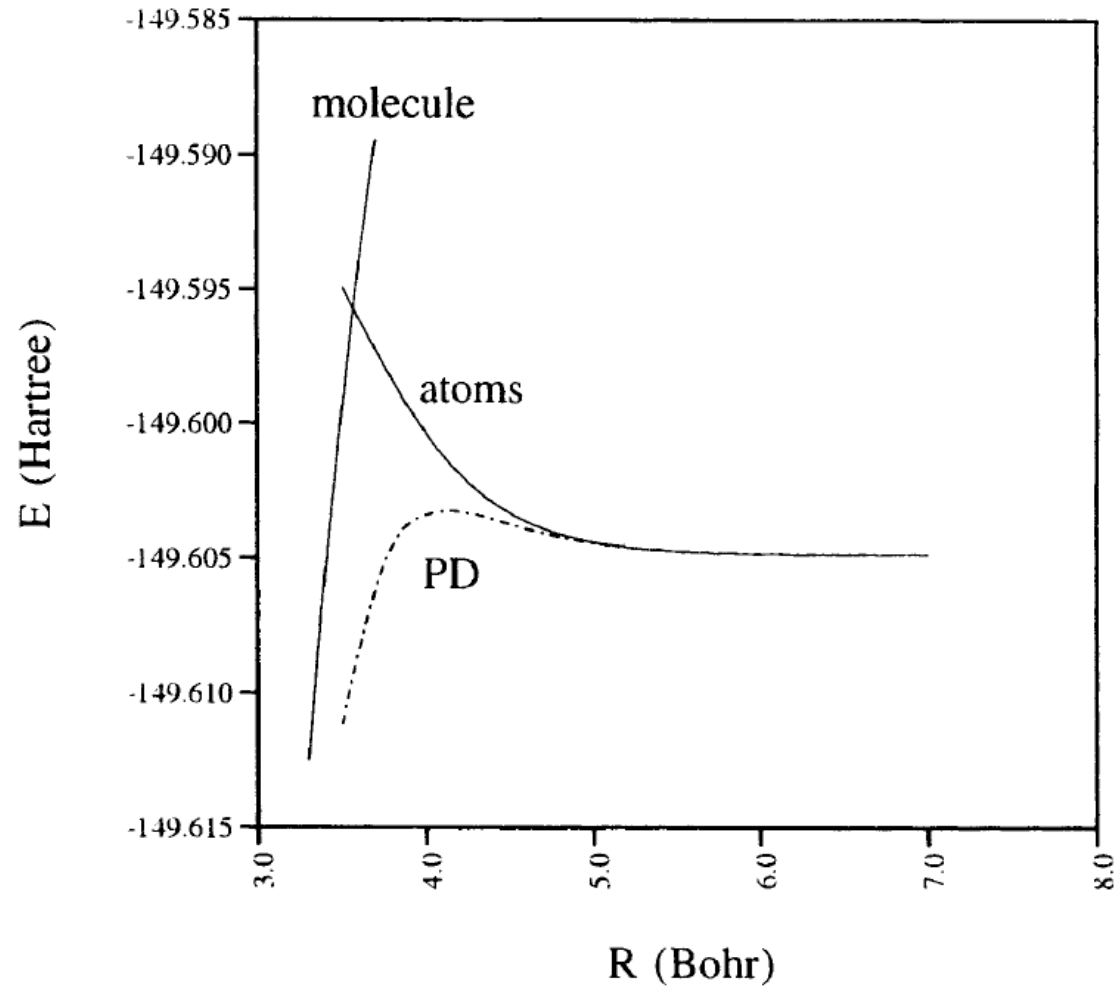


extra

Only valence
=> < 75 % of exp

At ∞ At R_e

Potential Energy Curve for O₂, with constituents parts



At least minimum comes later than expected, when the atoms approach