Recap on Basis Sets

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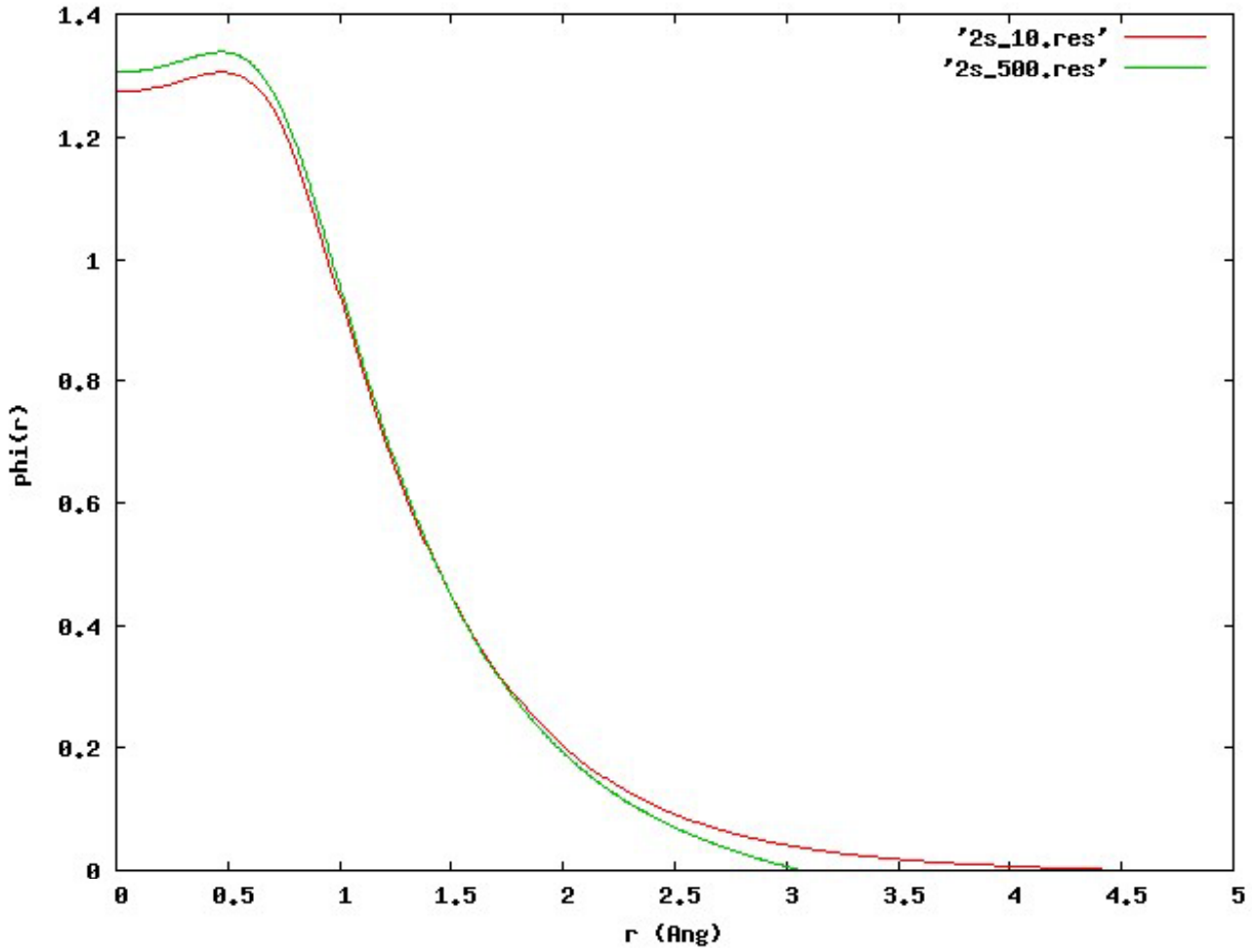
Basis Sets in SIESTA

- Generated from the solution of the FREE ATOM (with the pseudopotential)
- Finite range: $\varphi(r) = 0$ for $r \geq r_c$ (boundary condition)
- Energy shift by confinement:
  shorter r_c means higher energy $\rightarrow$ ΔE

Single-ζ (SZ)
and
First- ζ in MZ bases

Shape of the orbitals: r_c



O 2s orbital

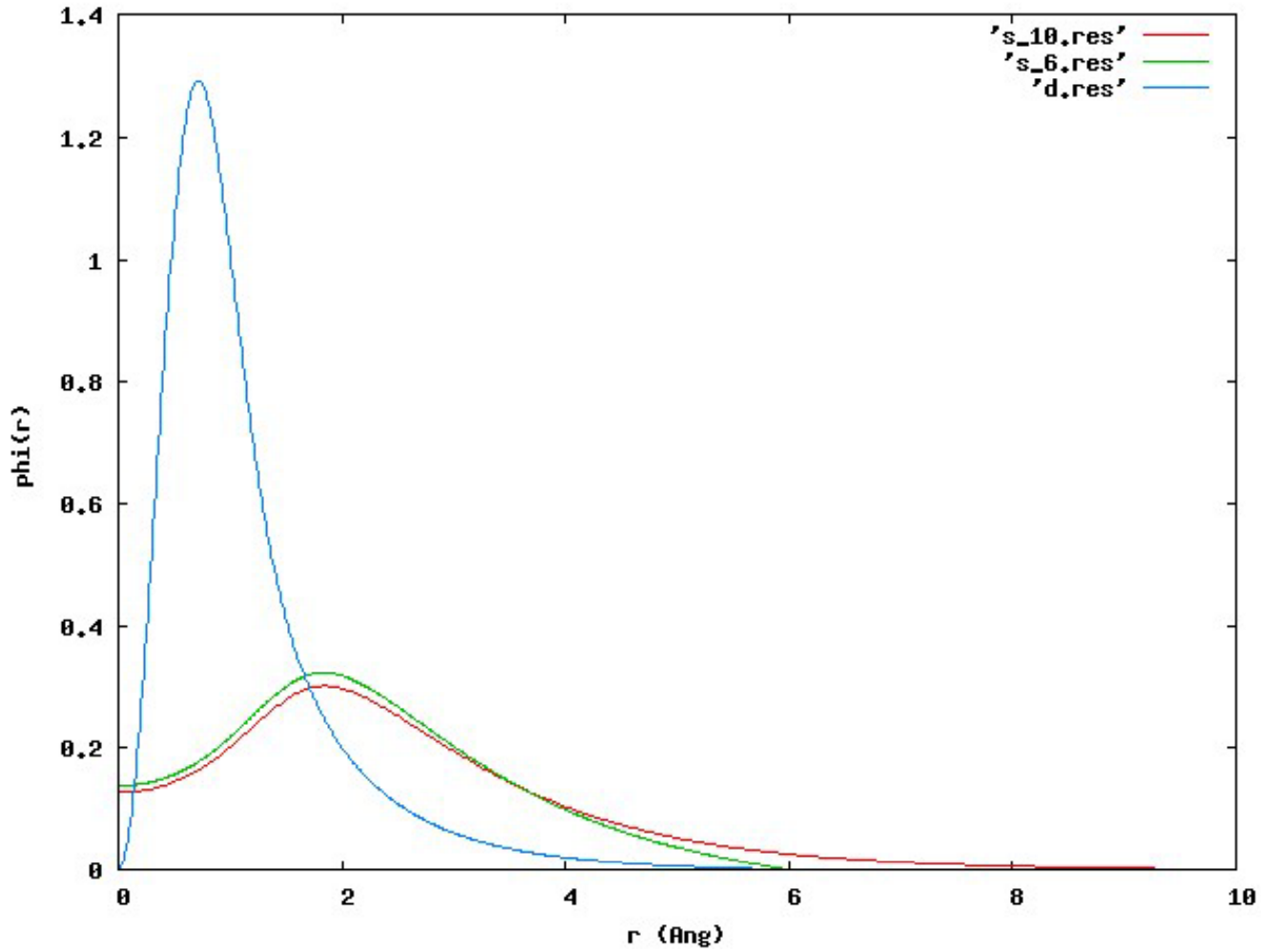
r_c = 3 a.u.

ΔE = 500 meV

r_c = 4.5 a.u.

ΔE = 10 meV

Shape of the orbitals: r_c



Fe 3d orbital

Fe 4s orbital

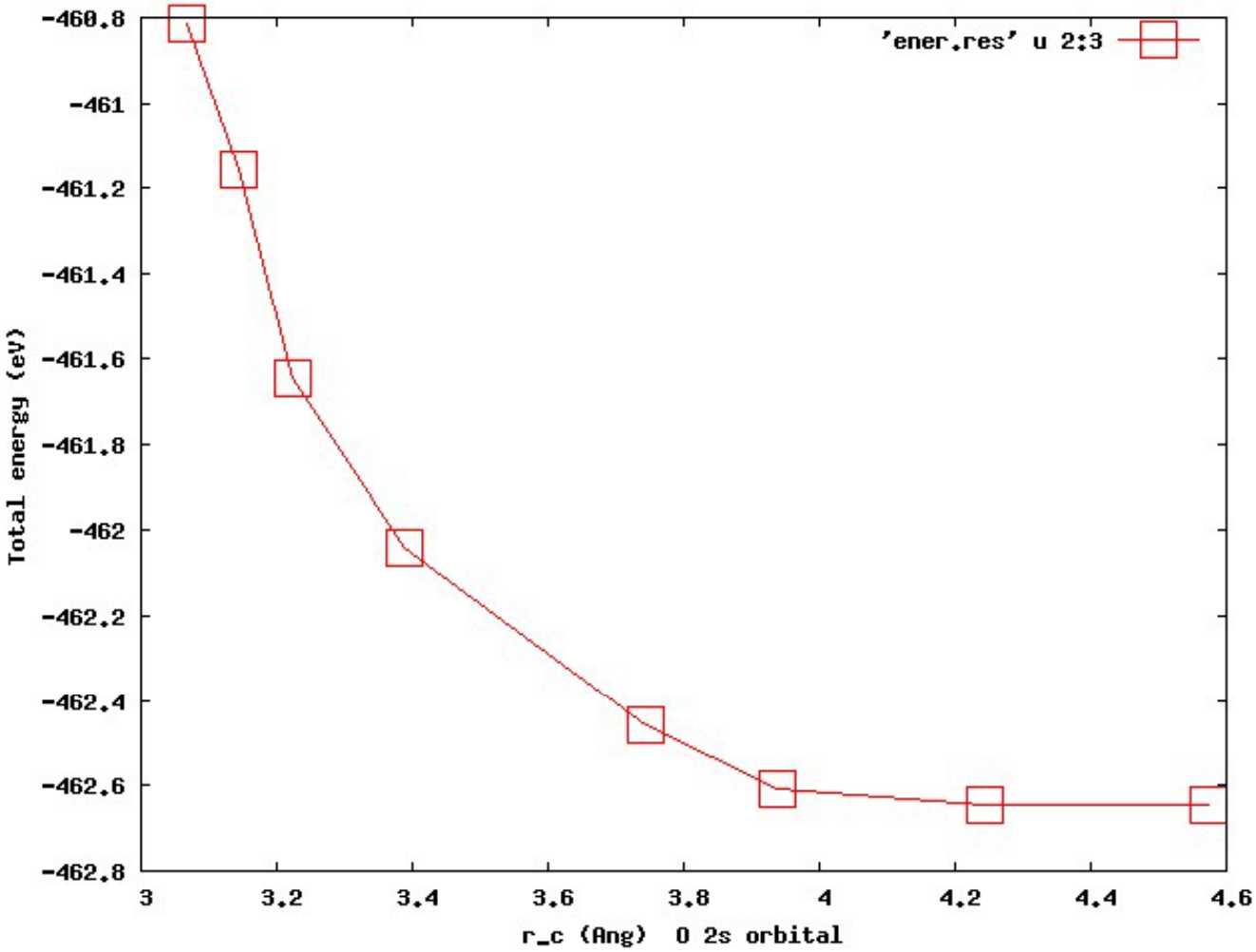
r_c = 6 a.u.

ΔE = 400 meV

r_c = 10 a.u.

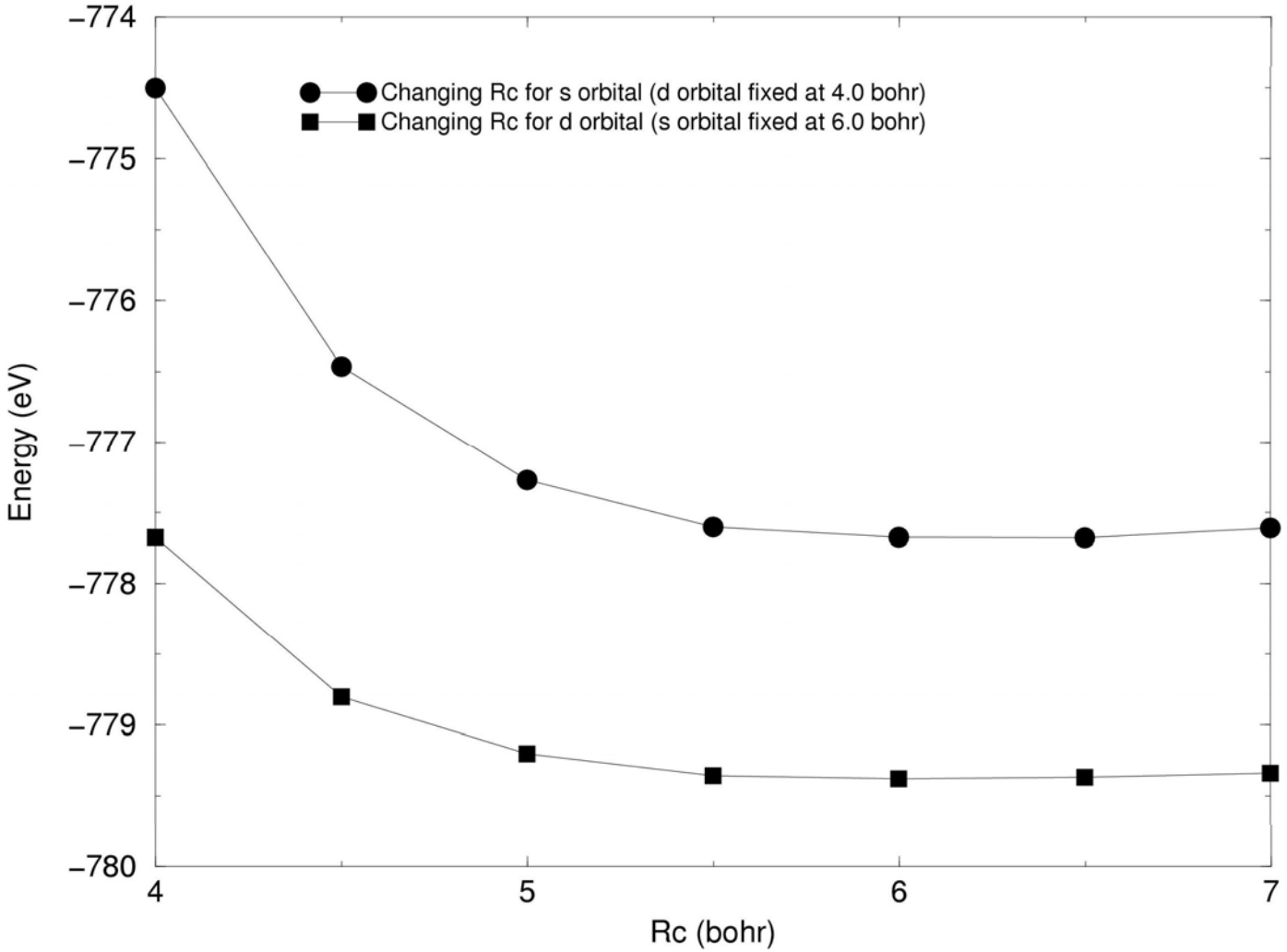
ΔE = 5 meV

Energy vs. r_c - Molecules



H_2O

Energy vs. r_c - Solids

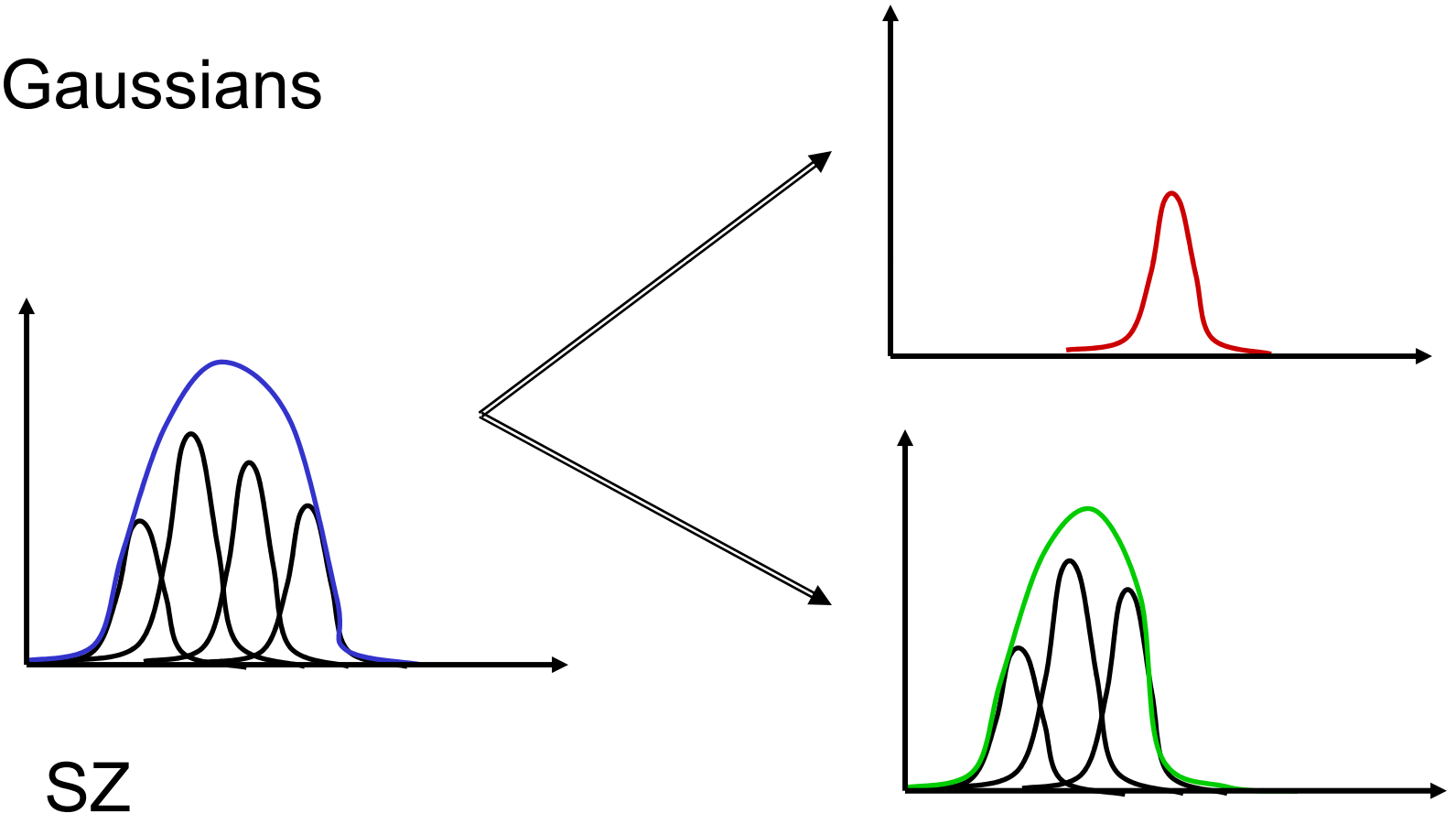


Bulk Fe

Second- ζ in DZ bases

Split Valence

Gaussians

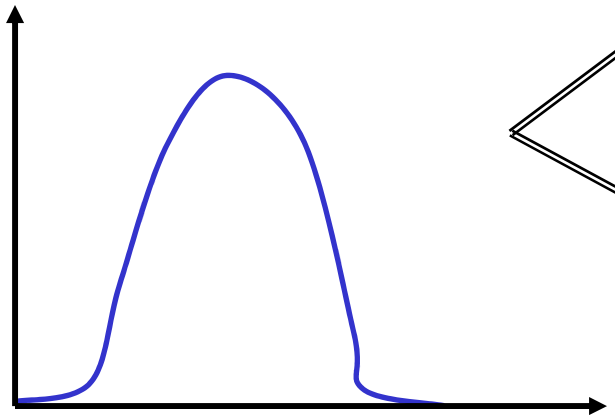


SZ

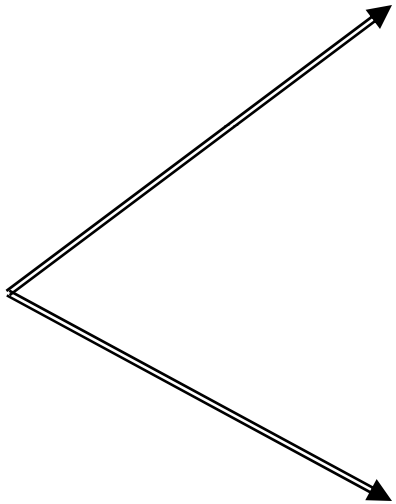
DZ

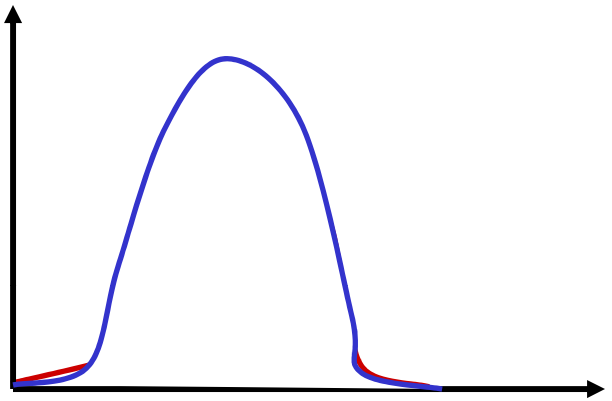
Split Valence

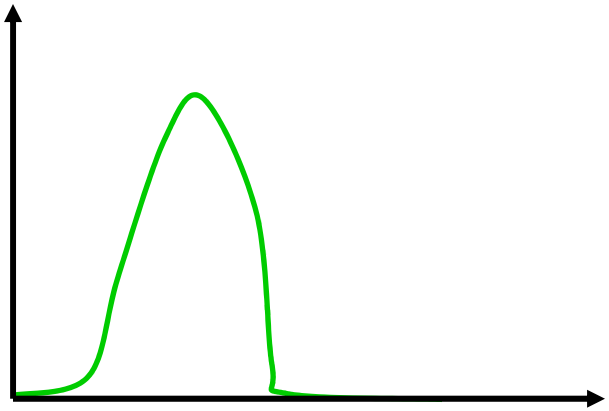
SIESTA



SZ

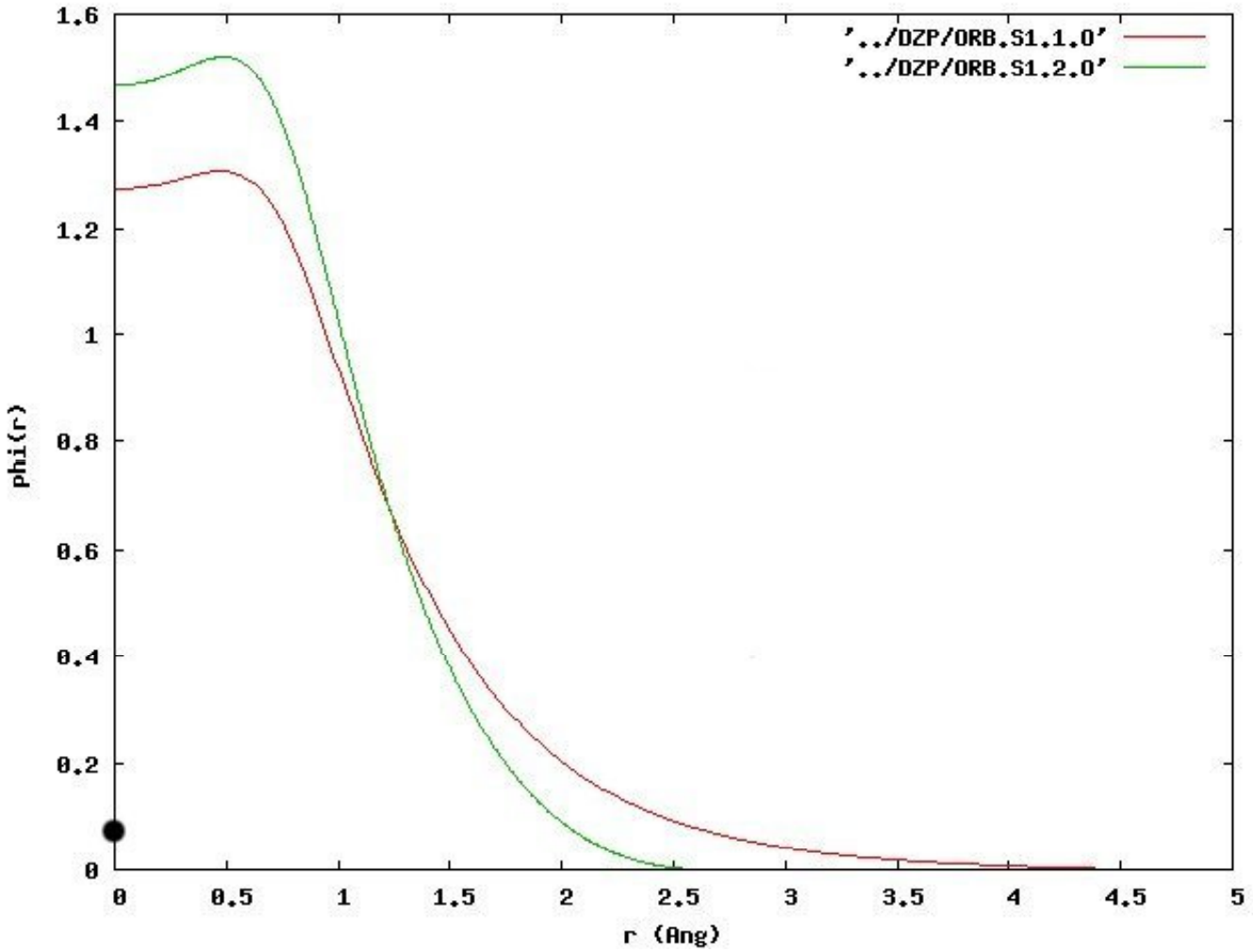






DZ

Shape of the orbitals: DZ

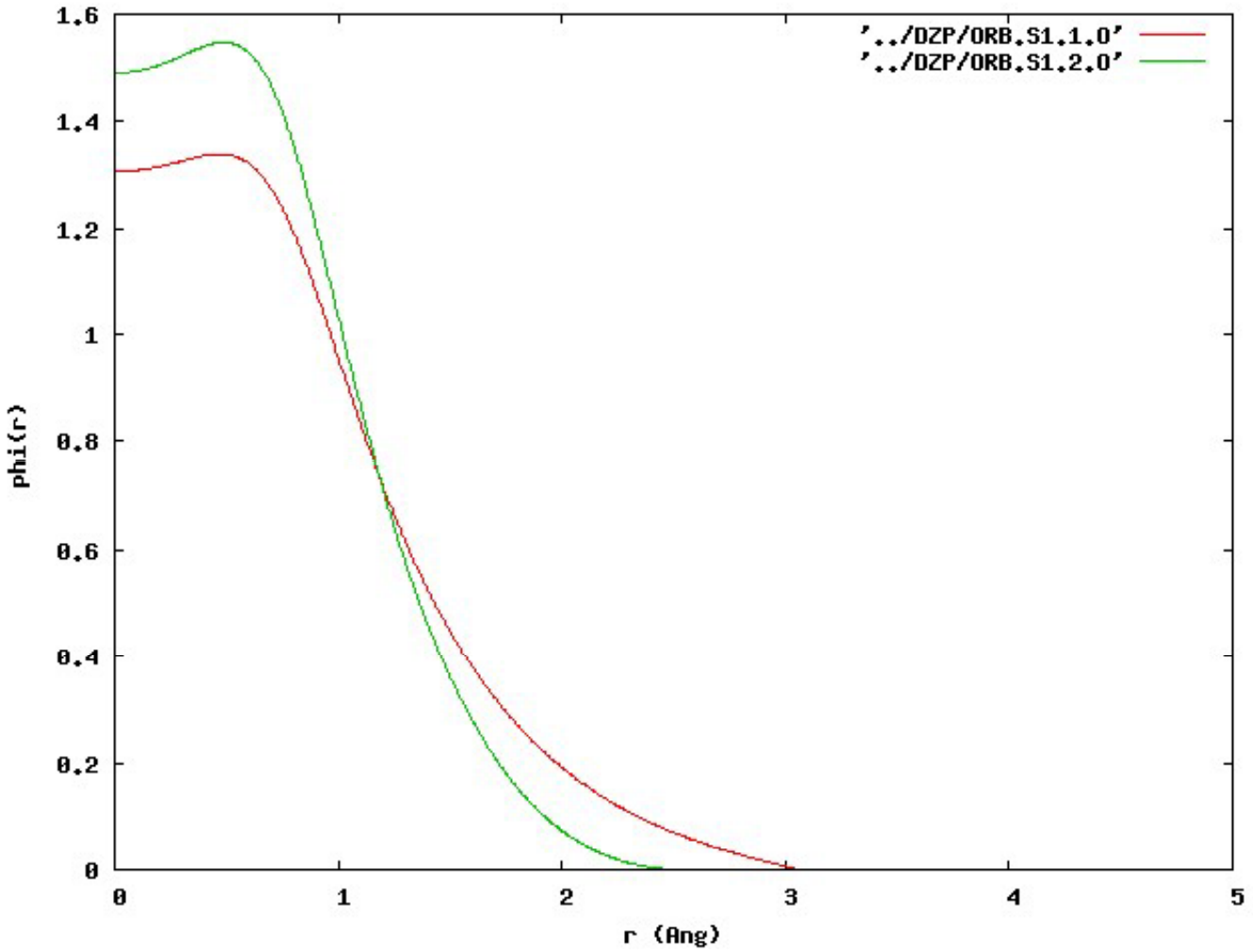


O 2s orbital

ΔE = 10 meV

SplitNorm 0.15

Shape of the orbitals: DZ



O 2s orbital

ΔE = 500 meV

SplitNorm 0.15