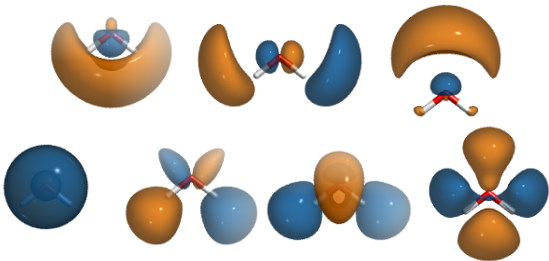
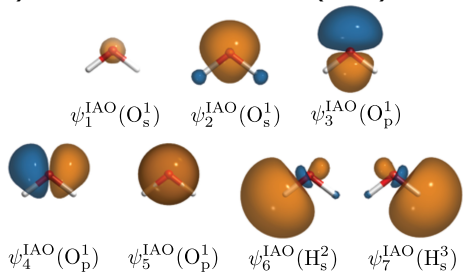


(A) Canonical molecular orbitals (CMOs)



(B) Intrinsic atomic orbitals (IAOs)

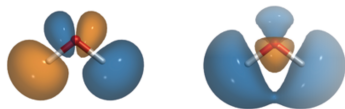


LIVO Procedure

(A) and (B)

SVD of overlap matrix

(C) Valence virtual orbitals (VVOs)



Pipek-Mezey
Localization

(D) Localized intrinsic VVOs (LIVOs)

