

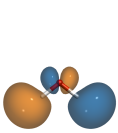






Percentage of Localized Intrinsic Valence Virtual Orbital Character


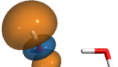
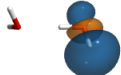
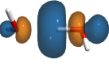
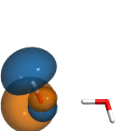
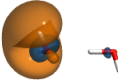

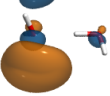
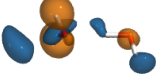
Particle Orbitals

(A) Water monomer

		 $\sigma_{\text{O}_1-\text{H}_2}^*$	 $\sigma_{\text{O}_1-\text{H}_3}^*$	Total Valence Character
	ϕ_{p}^1	42	42	85
	ϕ_{p}^2	38	38	75
	ϕ_{p}^3	0	0	0
	ϕ_{p}^4	0	0	0
	ϕ_{p}^5	6	6	12


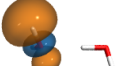

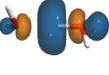
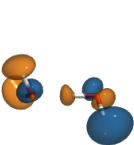



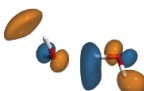
Particle Orbitals

(B) Water dimer-A

		 $\sigma_{\text{O}_1-\text{H}_2}^*$	 $\sigma_{\text{O}_1-\text{H}_3}^*$	 $\sigma_{\text{O}_4-\text{H}_6}^*$	 $\sigma_{\text{O}_4-\text{H}_5}^*$	Total Valence Character
	ϕ_{p}^1	41	41	0	0	84
	ϕ_{p}^2	39	39	0	0	77
	ϕ_{p}^3	0	0	9	14	23
	ϕ_{p}^4	0	0	4	3	7
	ϕ_{p}^5	4	4	12	8	29

Particle Orbitals

(C) Water dimer-D

		 $\sigma_{\text{O}_1-\text{H}_2}^*$	 $\sigma_{\text{O}_1-\text{H}_3}^*$	 $\sigma_{\text{O}_4-\text{H}_6}^*$	 $\sigma_{\text{O}_4-\text{H}_5}^*$	Total Valence Character
	ϕ_{p}^1	5	5	52	16	79
	ϕ_{p}^2	18	18	24	10	69
	ϕ_{p}^3	3	3	0	0	6
	ϕ_{p}^4	2	2	0	2	5
	ϕ_{p}^5	5	5	4	25	38