

H ₂ O	Experiment	DFT - PBE	Hartree-Fock	Δ -SCF (PBE)	Δ -SCF (HF)	$G_0 W_0$ @PBE	$G_0 W_0$ @HF	$G_0 W_0$ @PBE0
HOMO	12.615 eV							
HOMO-1	14.729 eV			***	***			
HOMO-2	18.550 eV			***	***			

Optional: C₂H₄

C ₂ H ₄	Experiment	DFT - PBE	Hartree-Fock	Δ -SCF (PBE)	Δ -SCF (HF)	$G_0 W_0$ @PBE	$G_0 W_0$ @HF	$G_0 W_0$ @PBE0
HOMO	10.68 eV							
HOMO-1	12.80 eV			***	***			
HOMO-2	14.80 eV			***	***			
HOMO-3	16.0 eV			***	***			