

Spin density and molecular orbital figures

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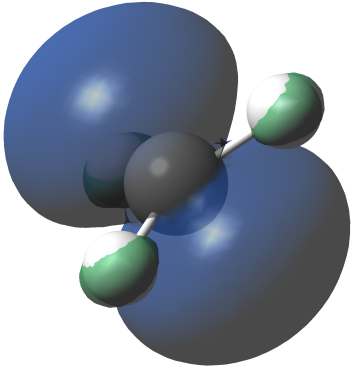
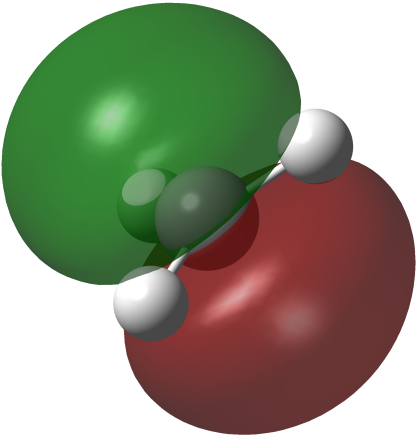
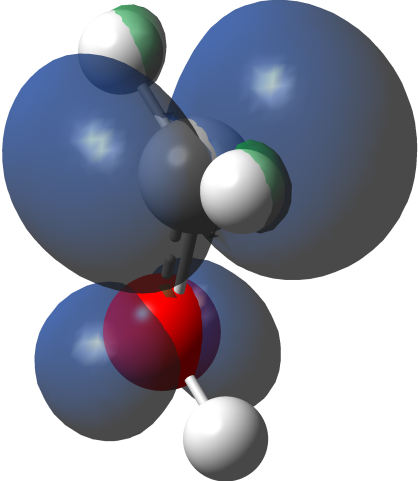
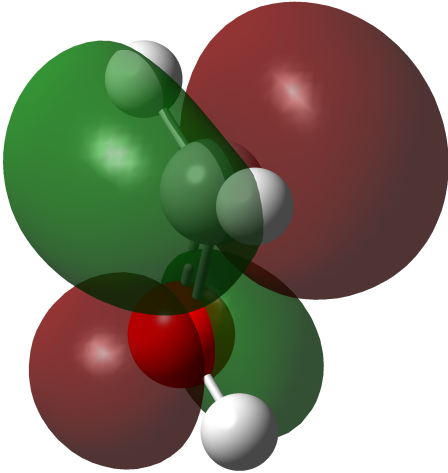
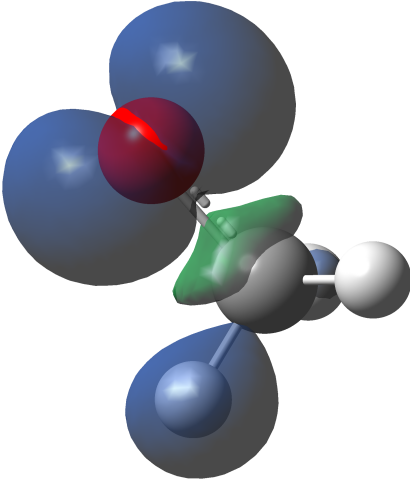
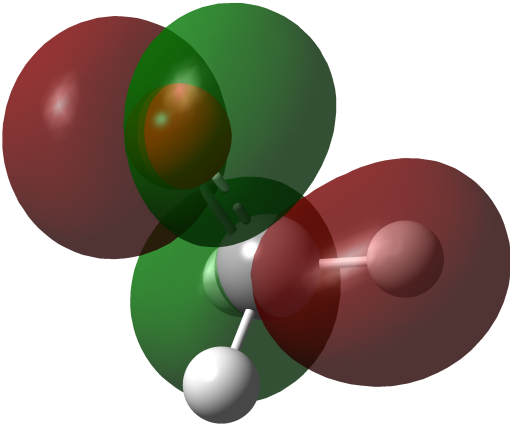
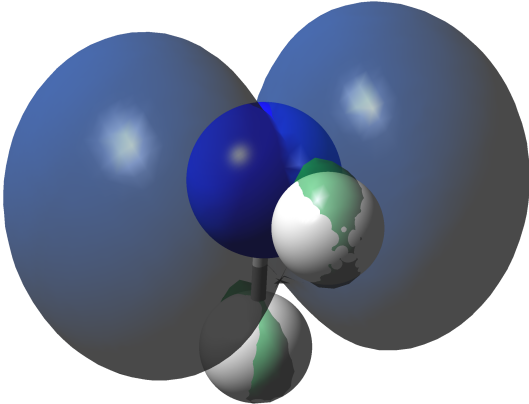
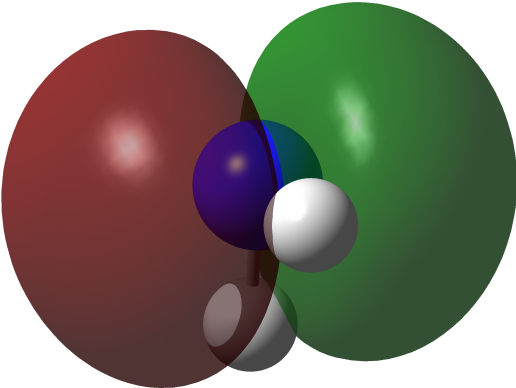
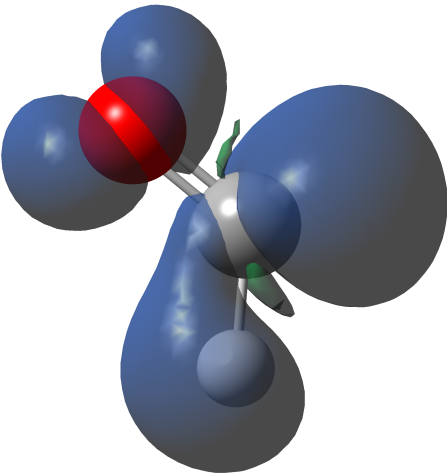
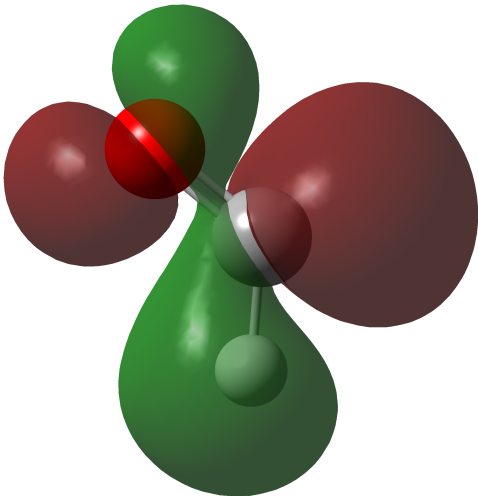
Reactants on W33 ... 17

TS on W33 ... 21

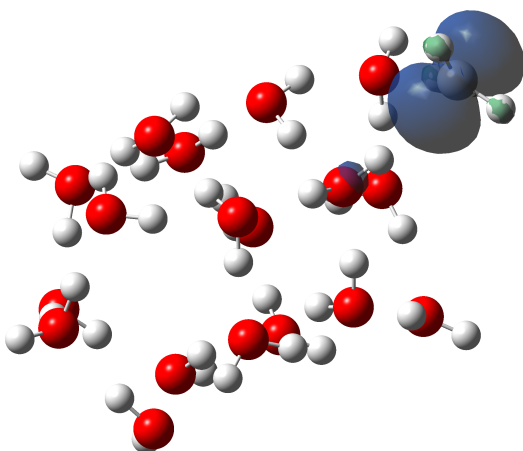
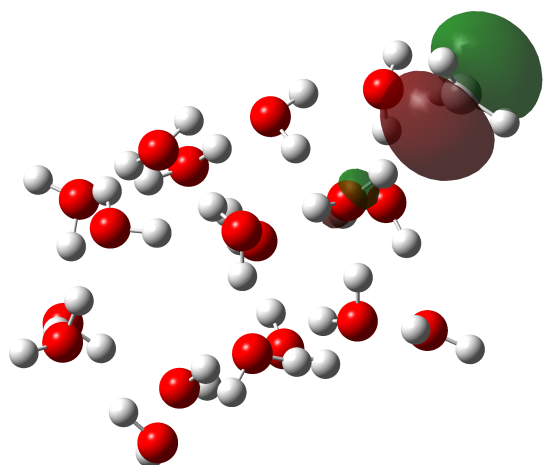
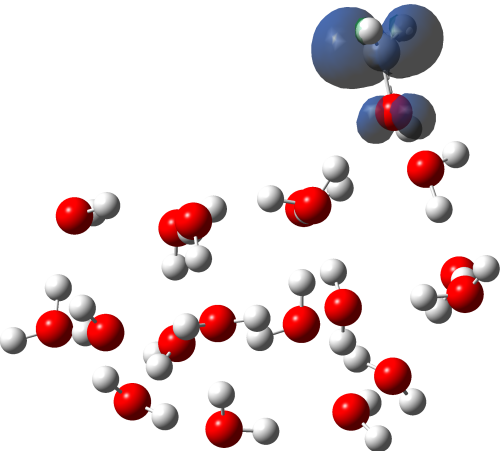
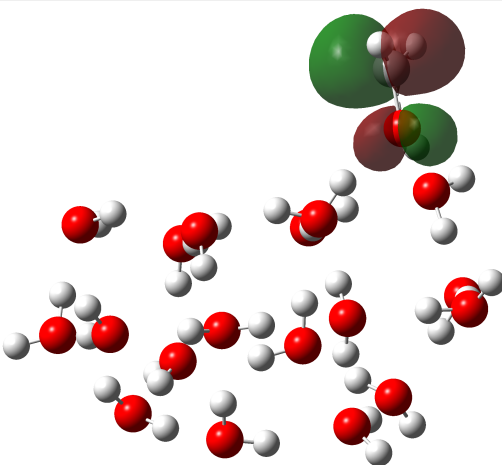
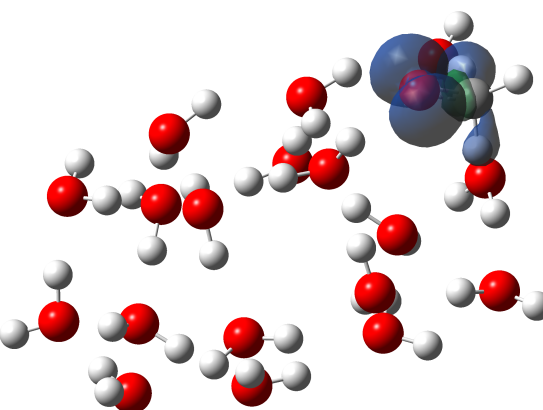
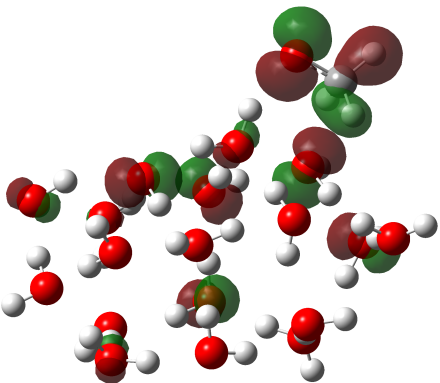
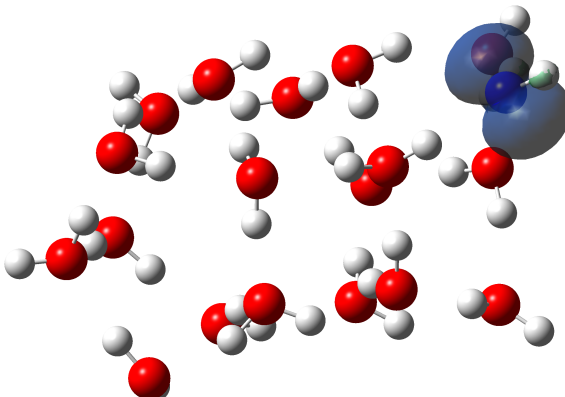
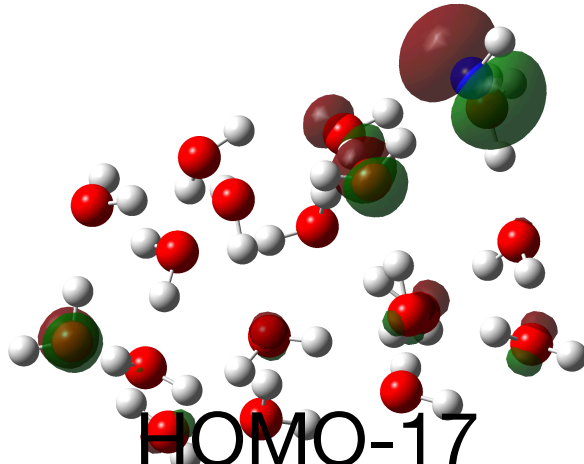
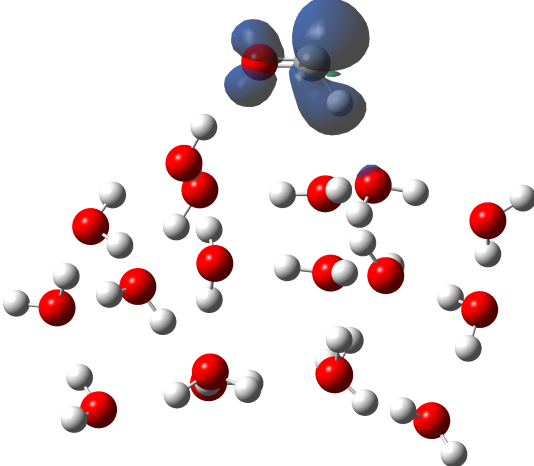
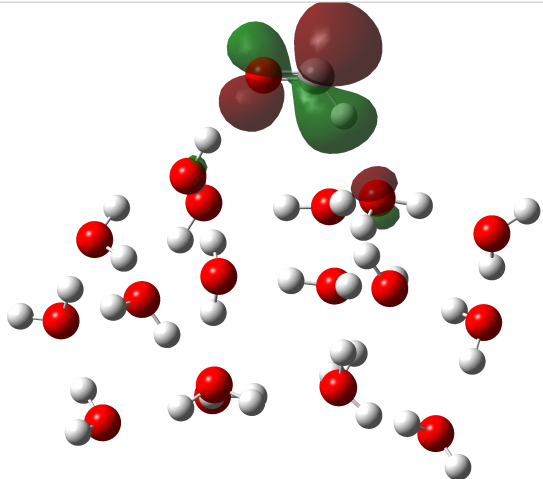
Notes:

- SD = Spin density
- SOMO = Singly occupied molecular orbital
- α MO = alpha molecular orbital (the one of the SOMO of the radical with positive spin density)
- β MO = beta molecular orbital (the one of the SOMO of the radical with negative spin density)
- The isovalue for density was chosen to be 0.004, and 0.04 for the MOs.

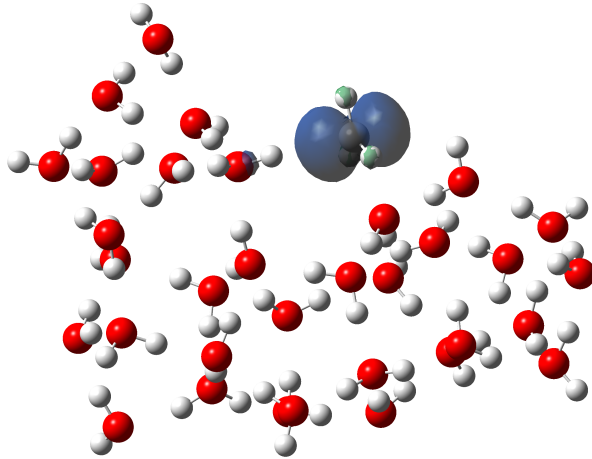
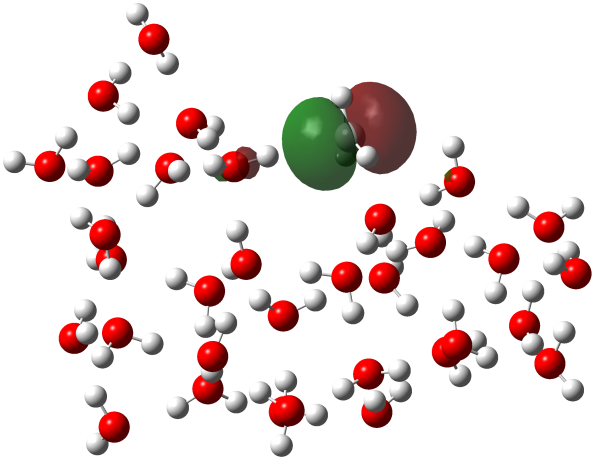
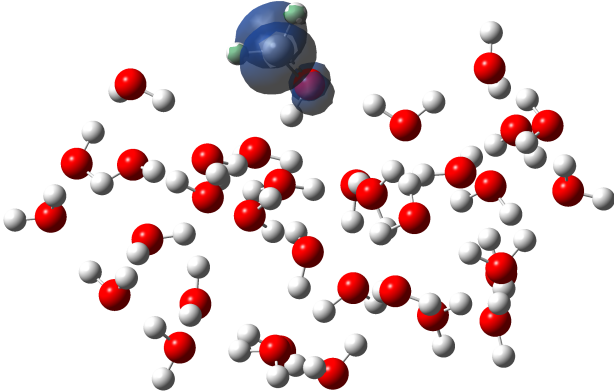
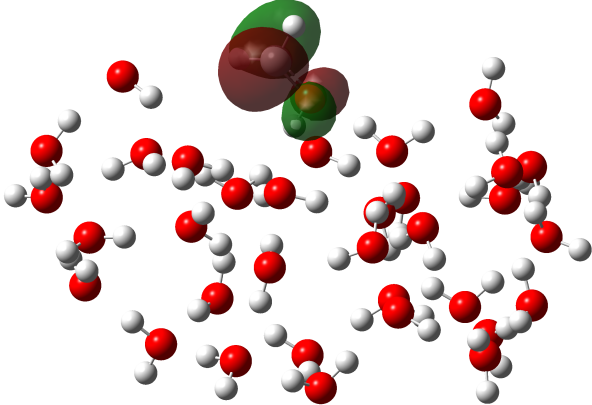
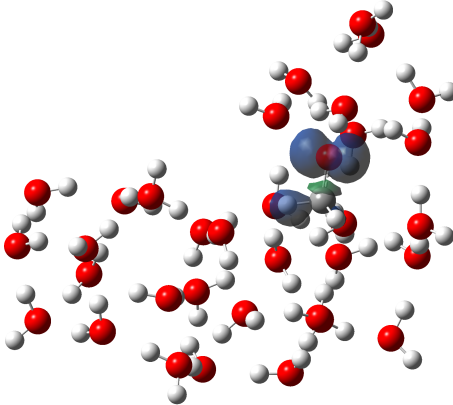
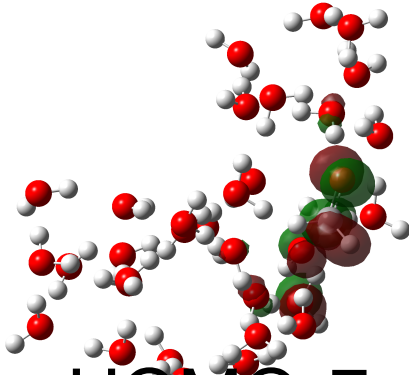
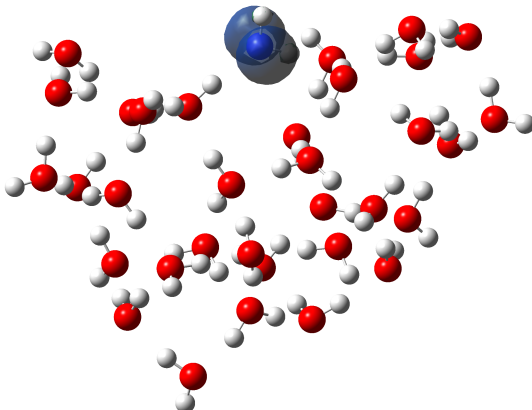
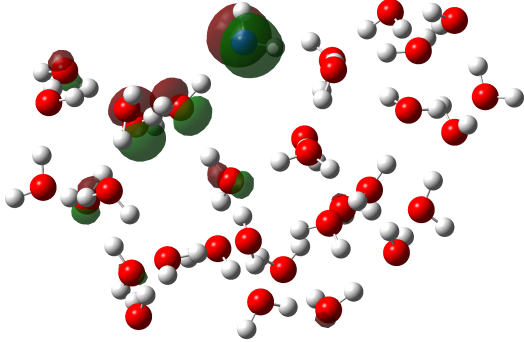
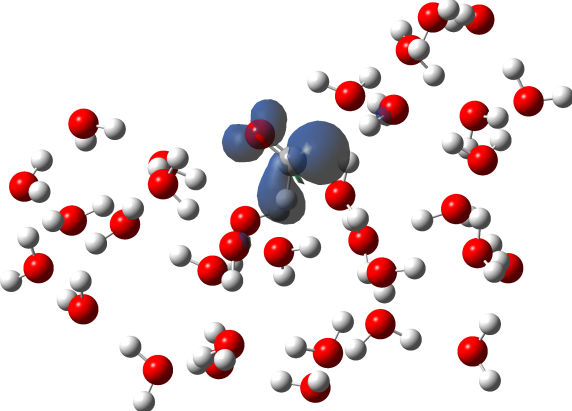
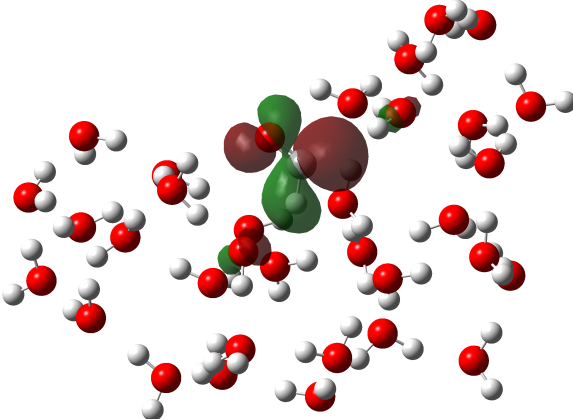
Isolated radicals

System	SD	SOMO
CH3		
CH2OH		
CH3O		
NH2		
HCO		

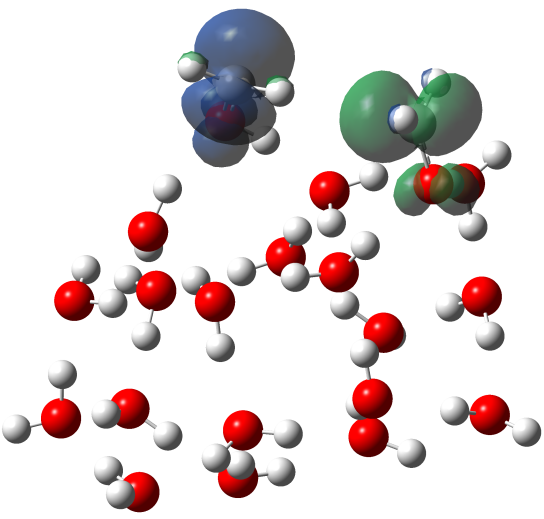
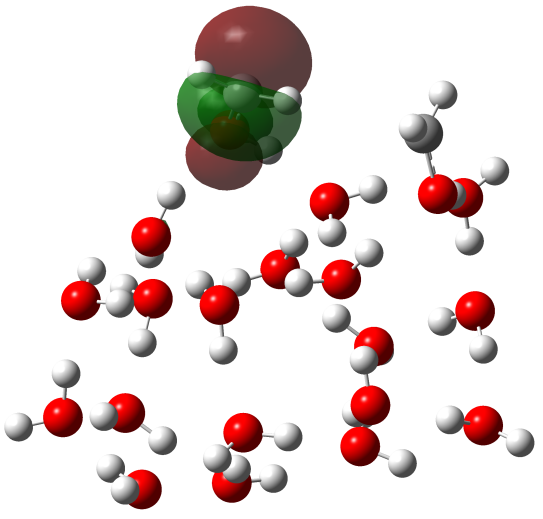
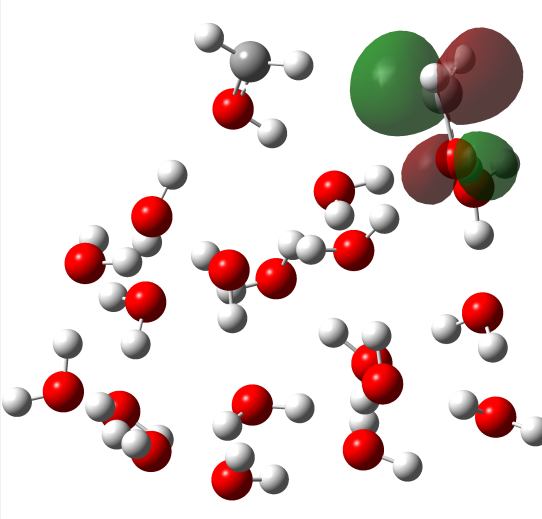
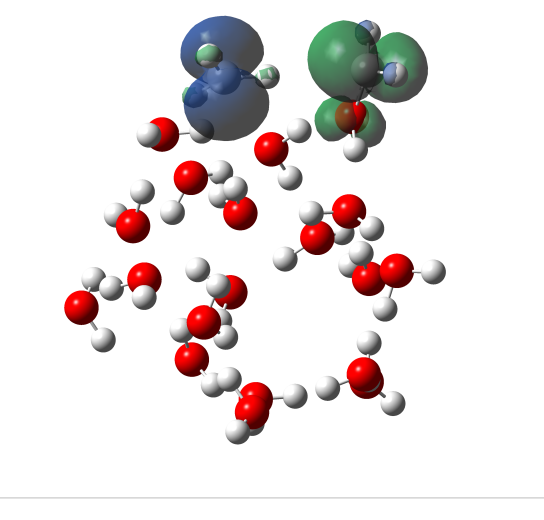
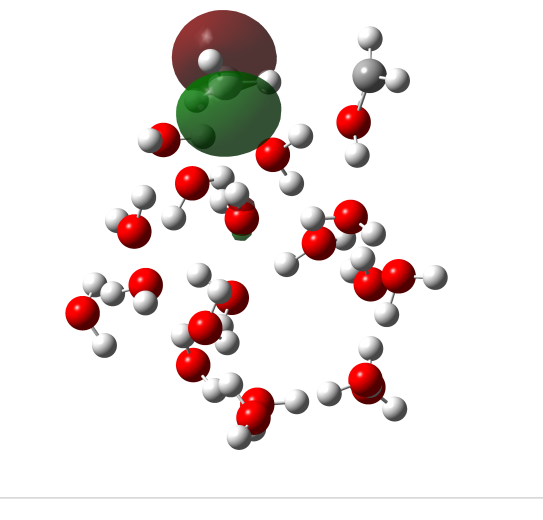
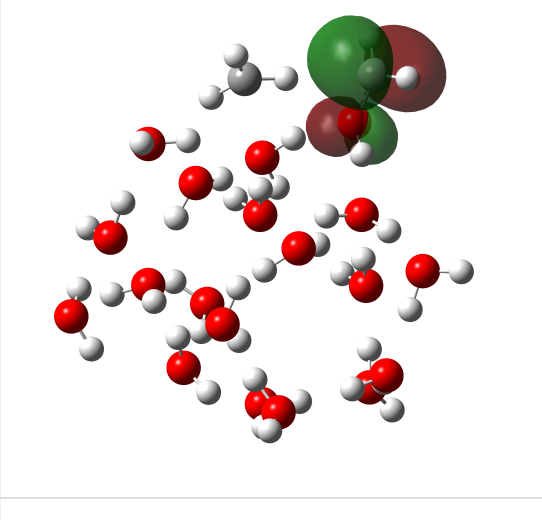
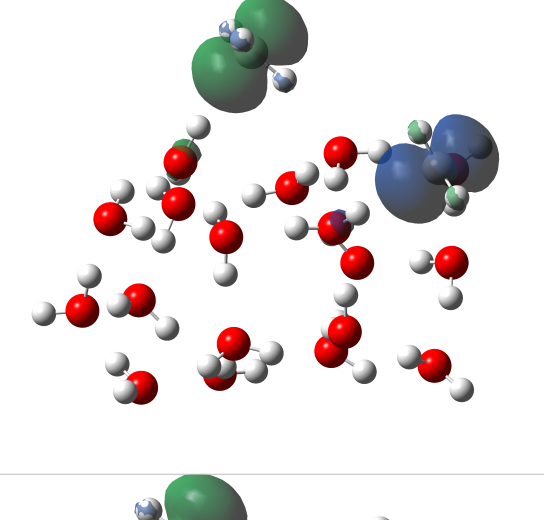
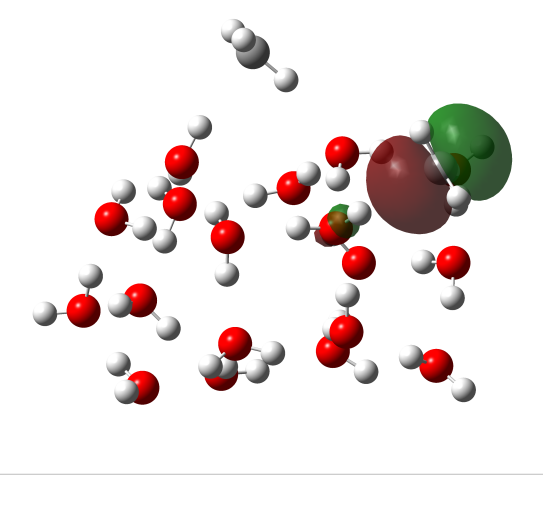
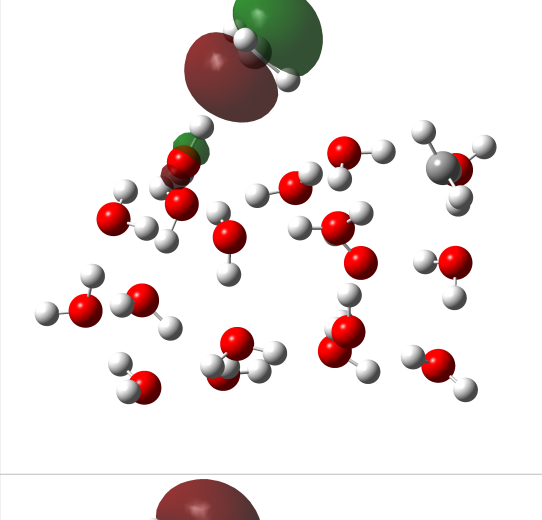
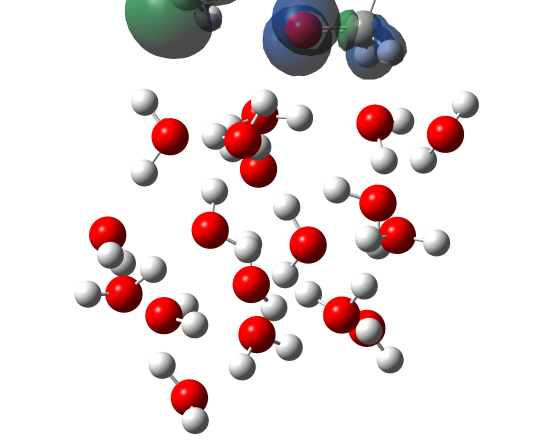
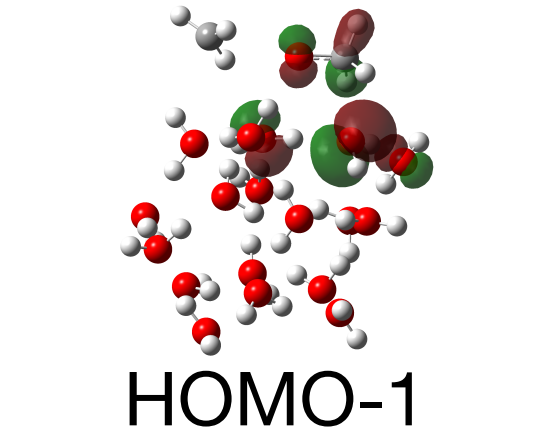
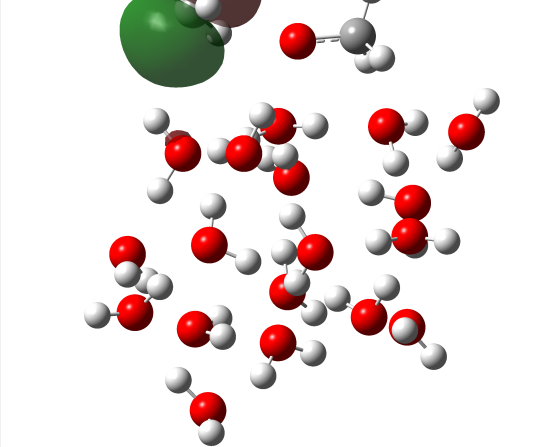
Adsorbed on W18

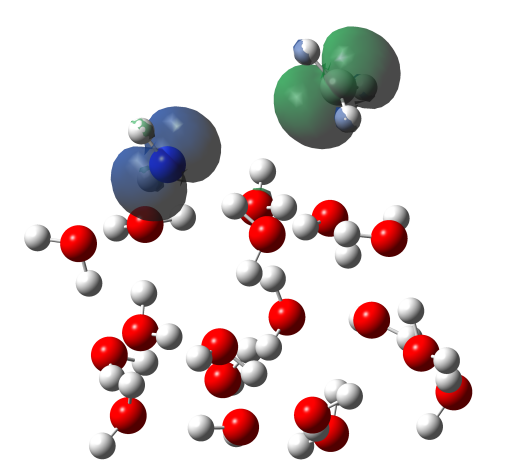
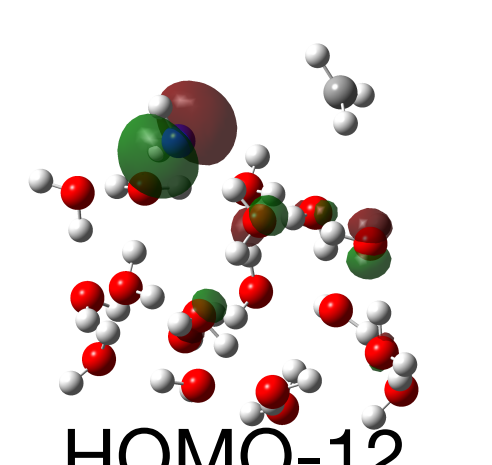
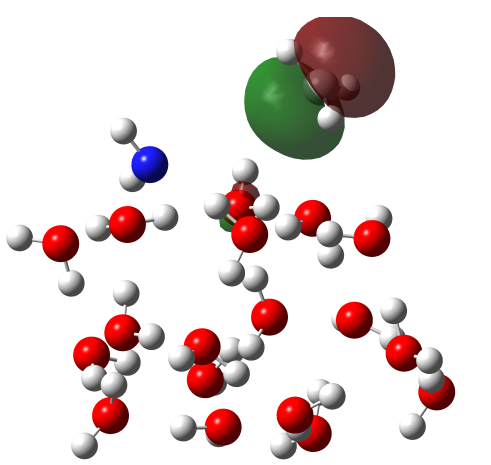
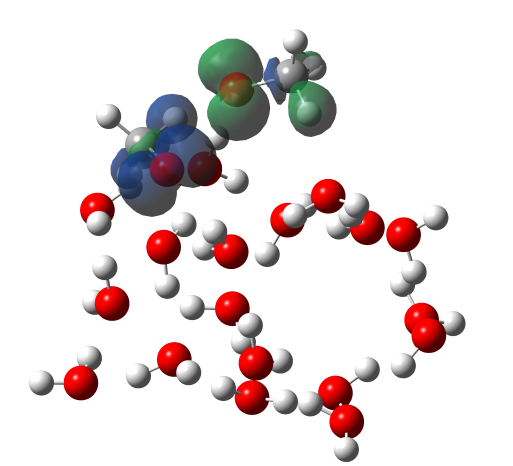
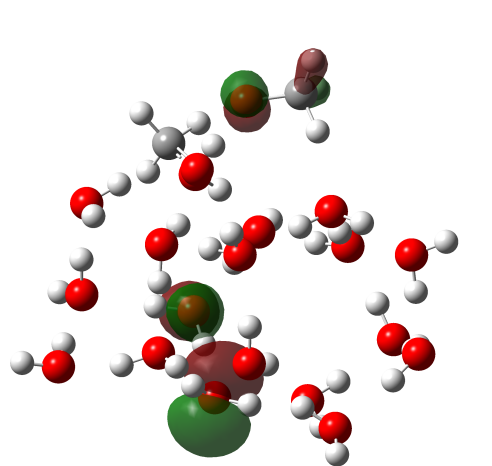
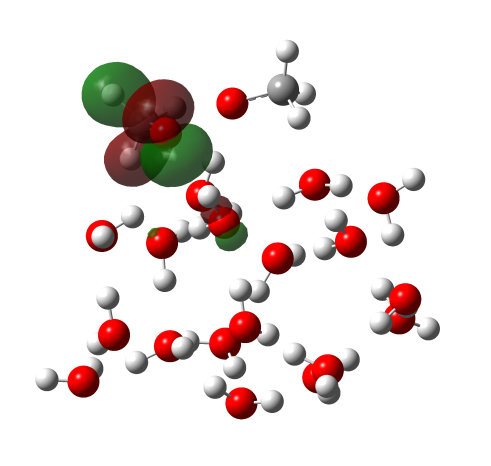
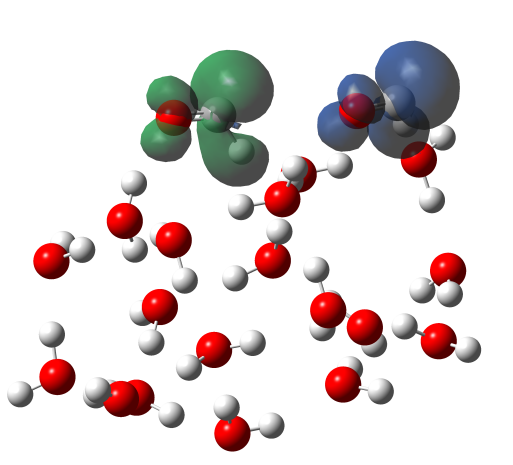
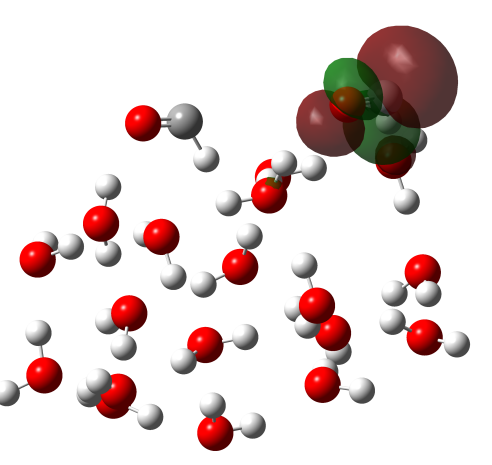
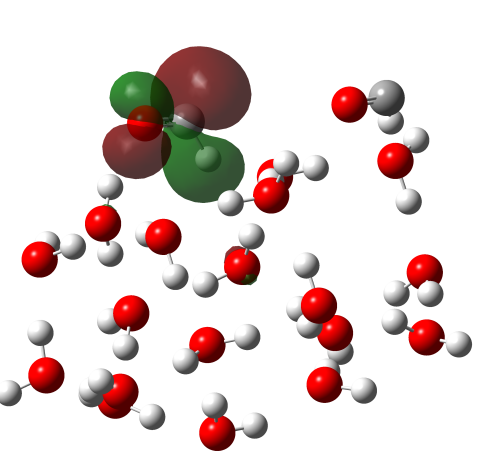
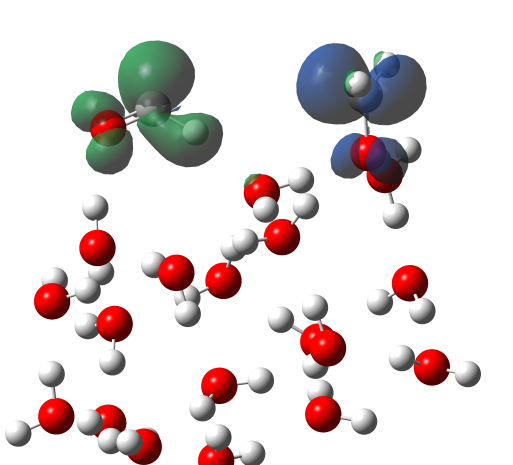
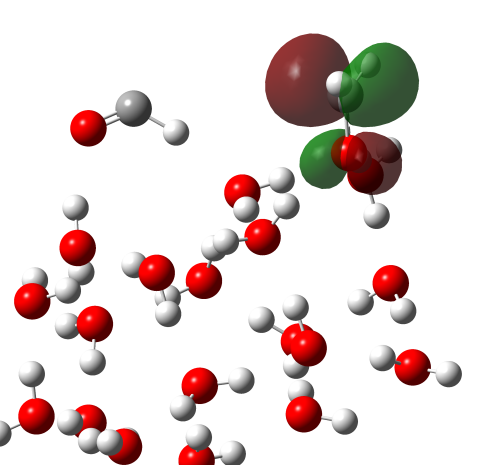
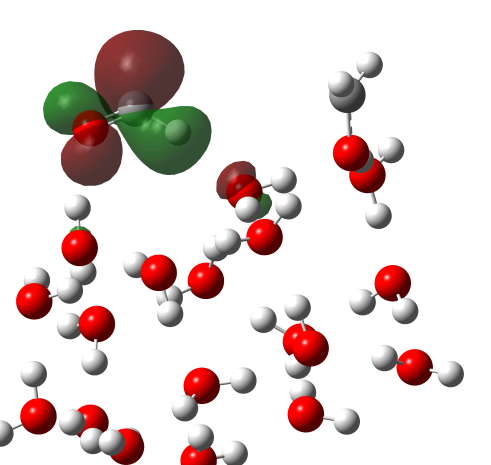
System	SD	SOMO
CH3		
CH2OH		
CH3O		 HOMO-1
NH2		 HOMO-17
HCO		

Adsorbed on W33

System	SD	SOMO
CH3		
CH2OH		
CH3O		 HOMO-7
NH2		 HOMO-33
HCO		

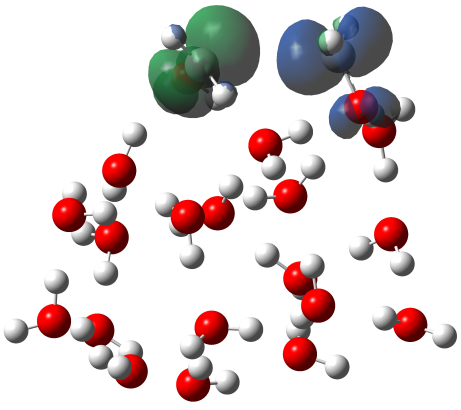
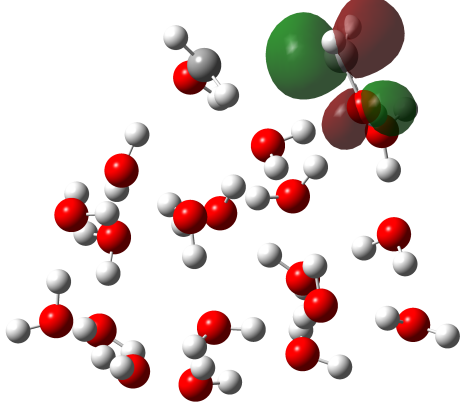
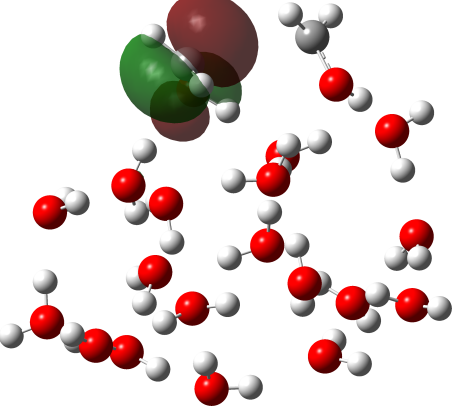
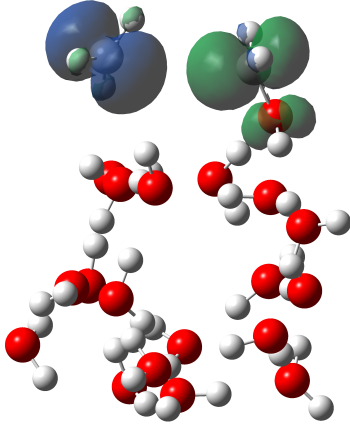
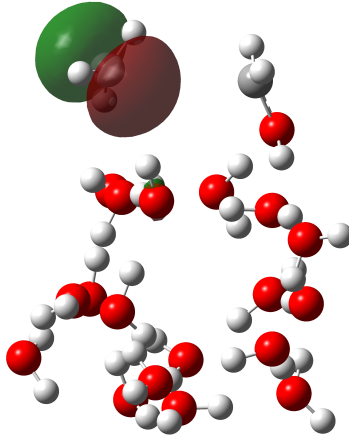
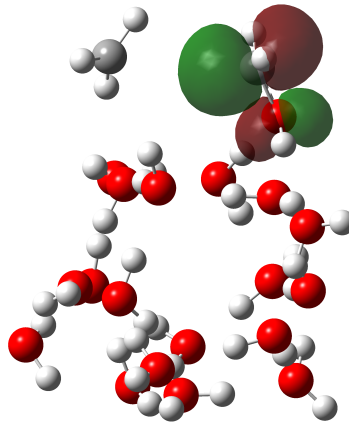
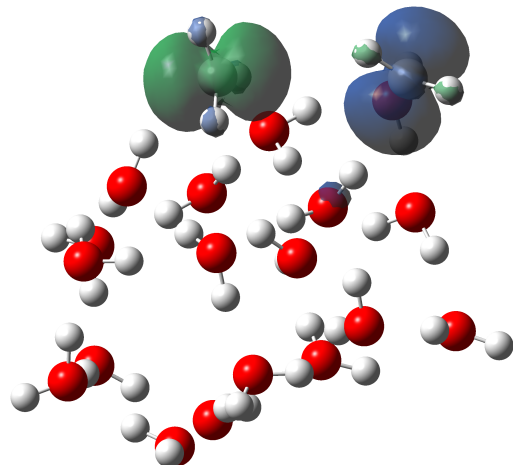
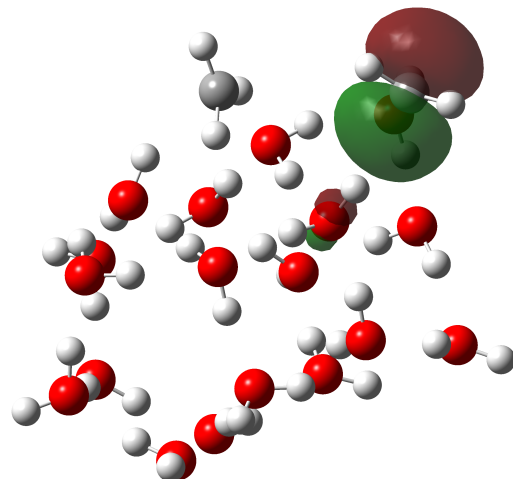
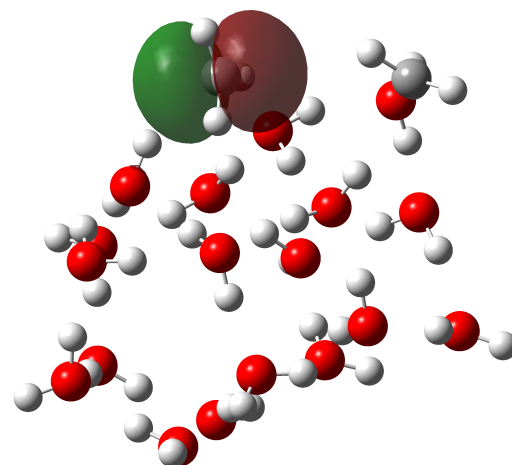
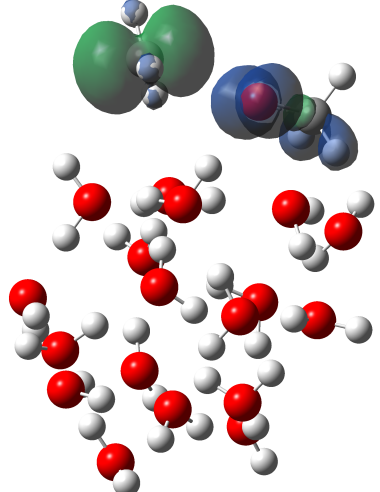
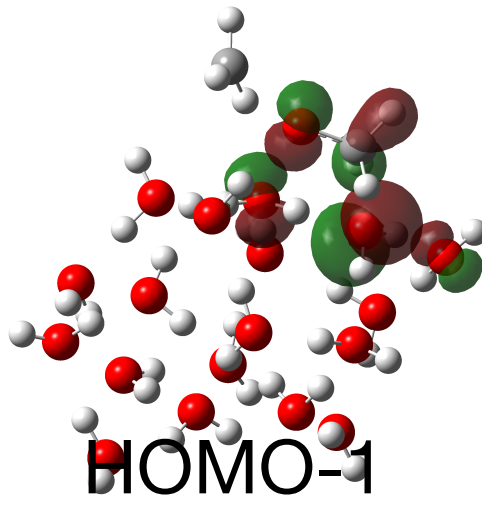
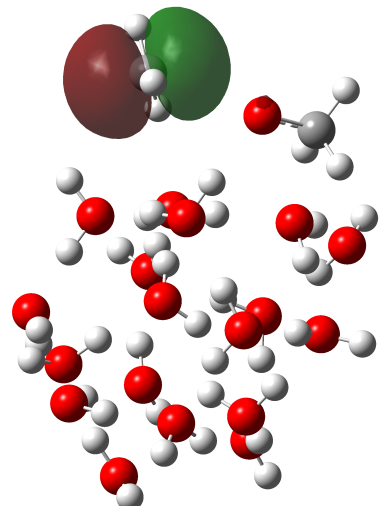
Reactants on W18

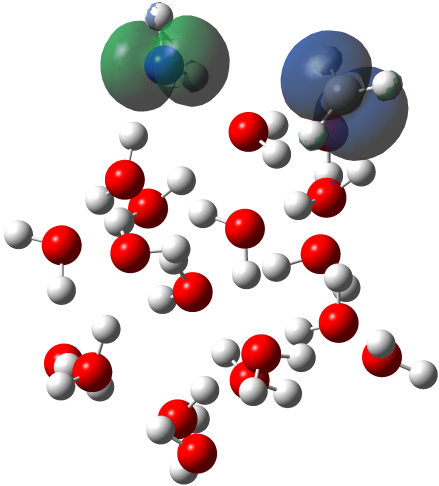
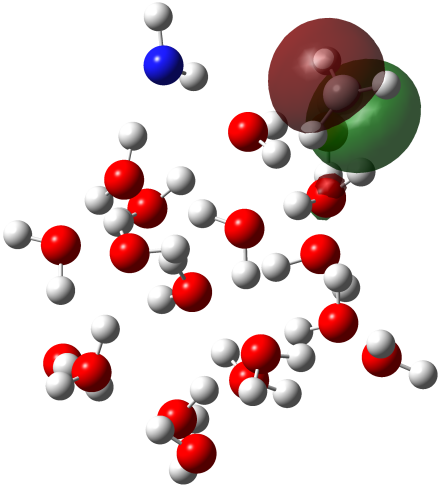
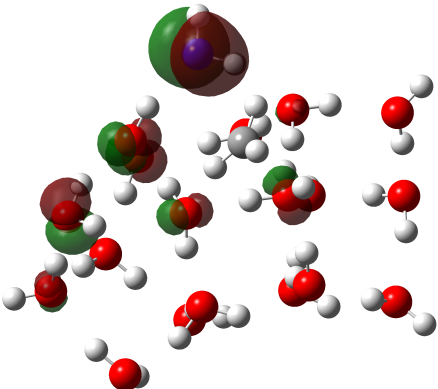
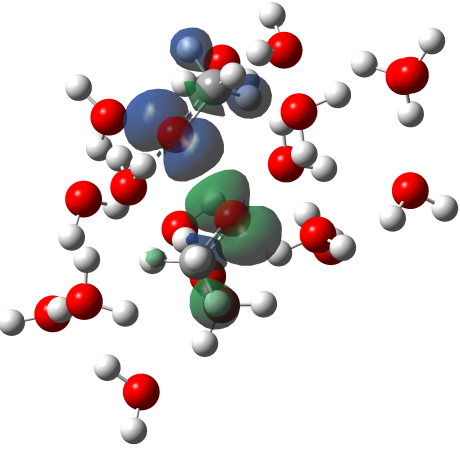
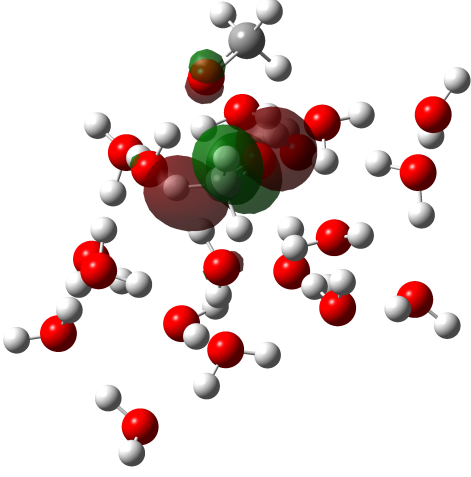
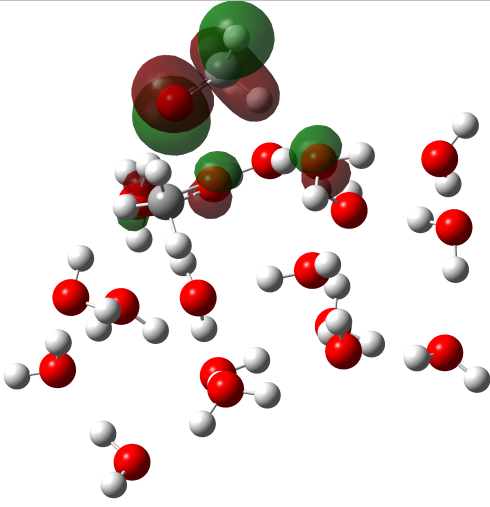
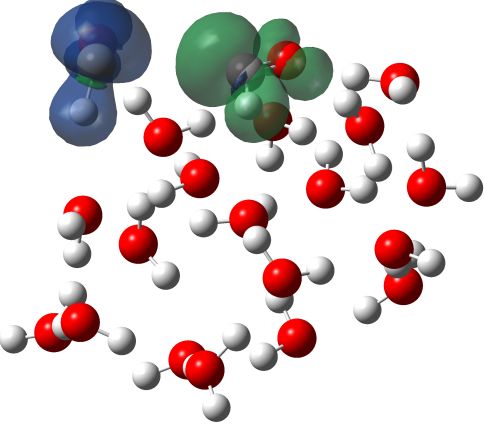
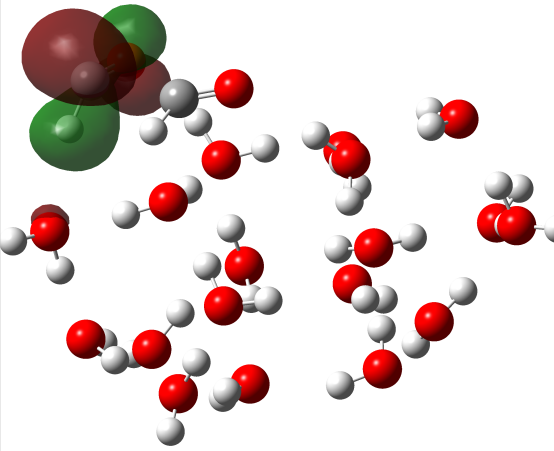
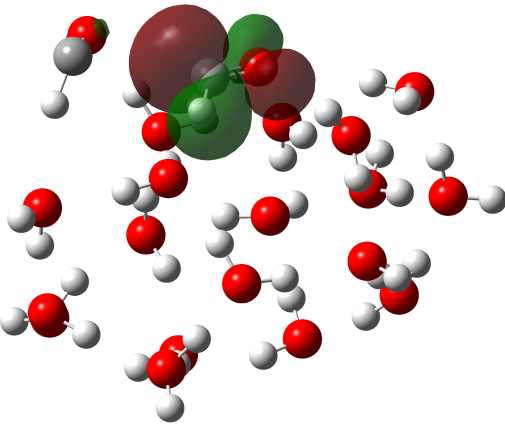
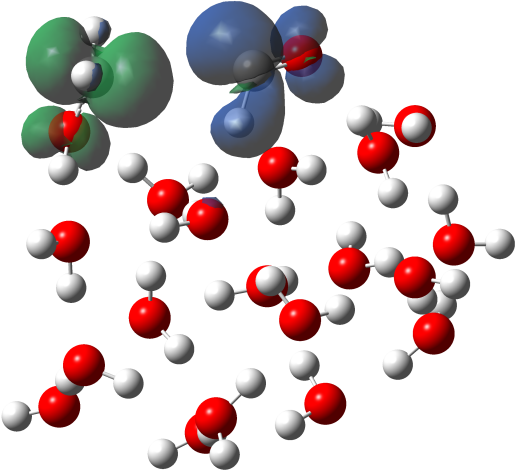
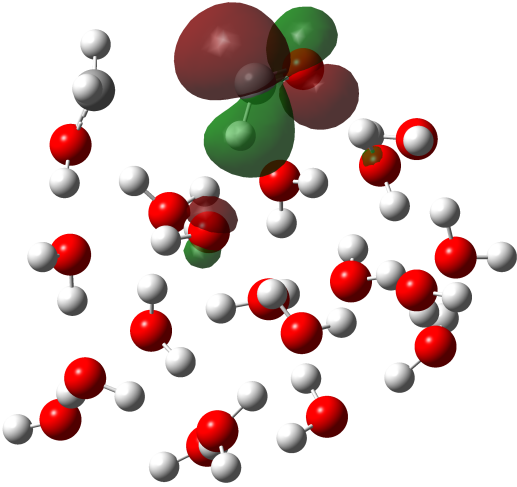
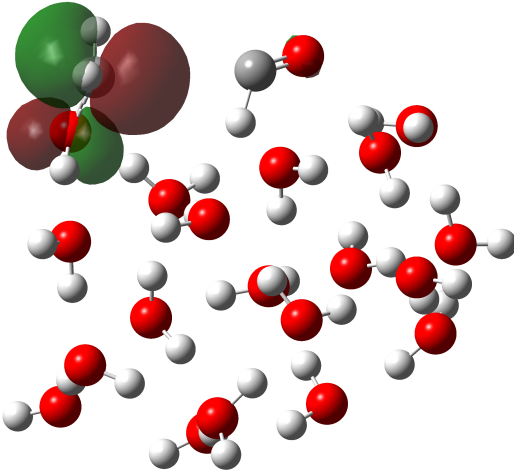
System	SD	α MO	β MO
CH₂OH + CH₂OH			
CH₃ + CH₂OH			
CH₃ + CH₃			
CH₃ + CH₃O		 HOMO-1	

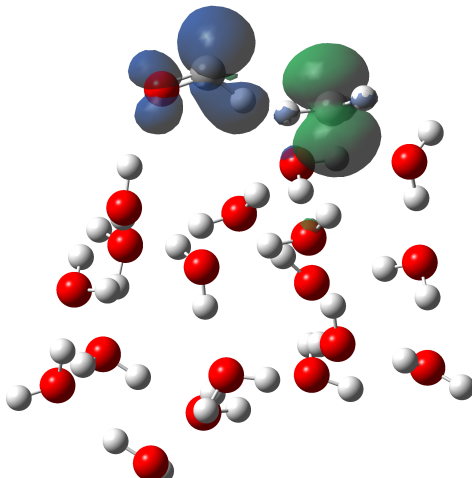
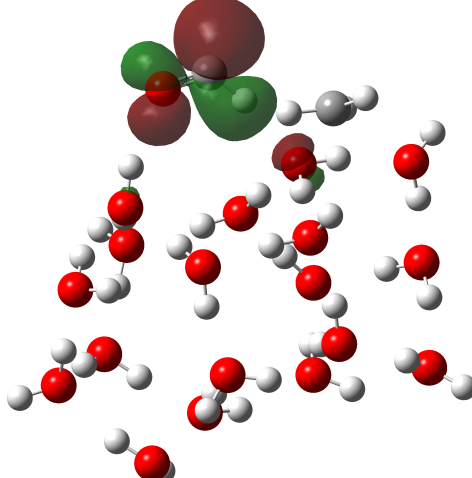
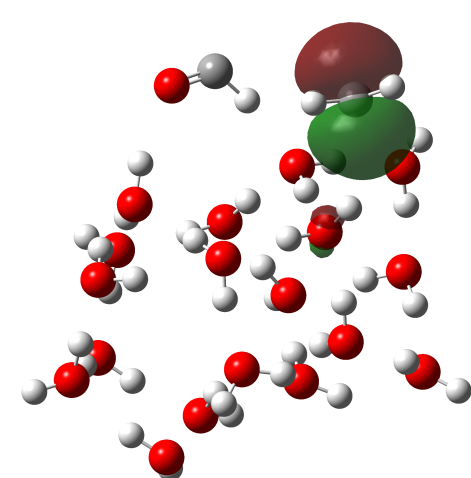
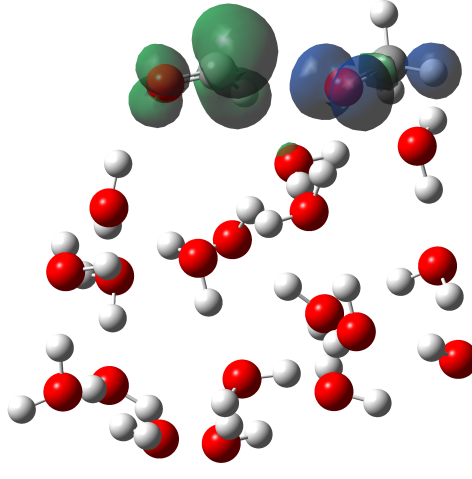
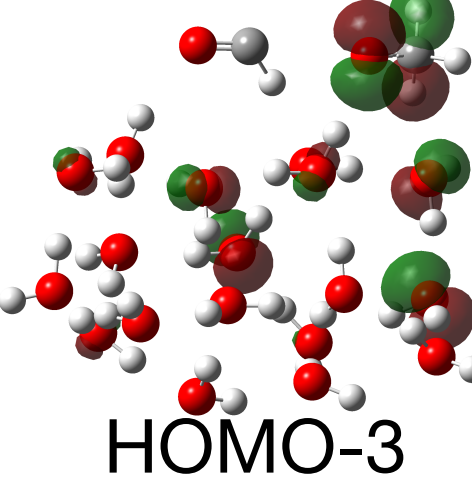
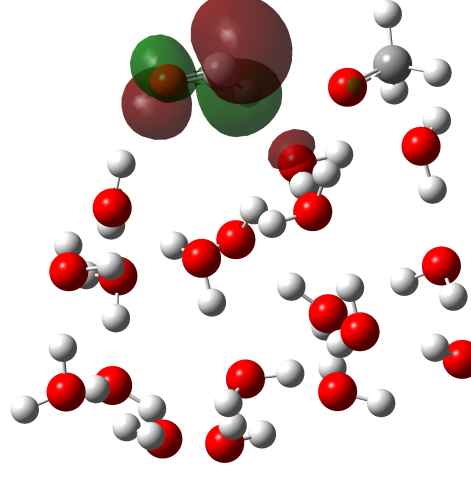
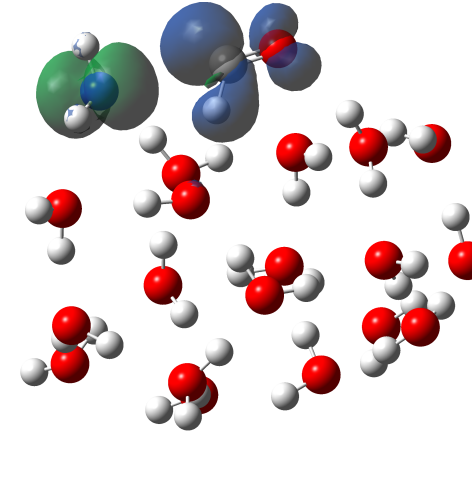
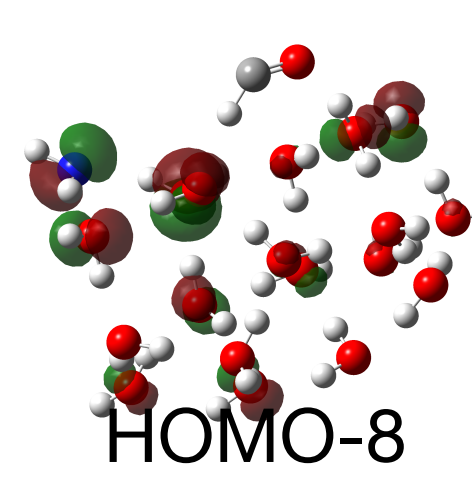
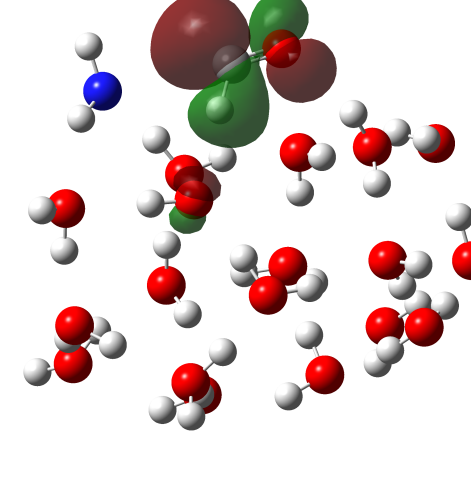
System	SD	α MO	β MO
CH ₃ + NH ₂		 HOMO-12	
CH ₃ O + CH ₃ O			
HCO + HCO			
HCO + CH ₂ OH			

System	SD	α MO	β MO
CH ₃ + HCO			
HCO + CH ₃ O			
HCO + NH ₂			

TS on W18

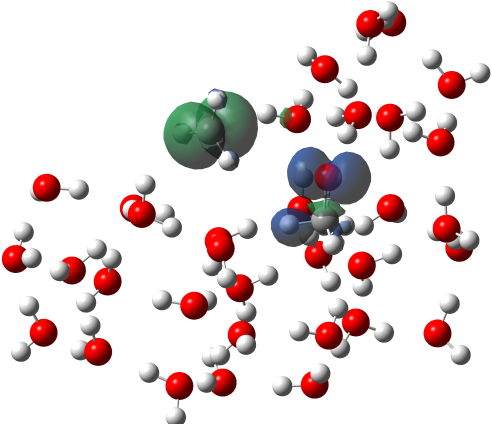
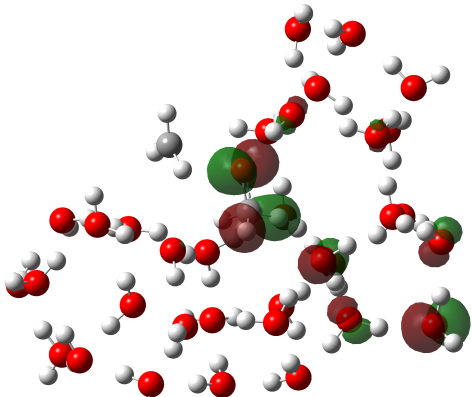
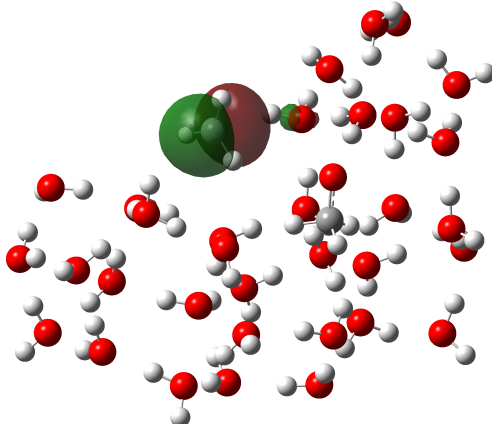
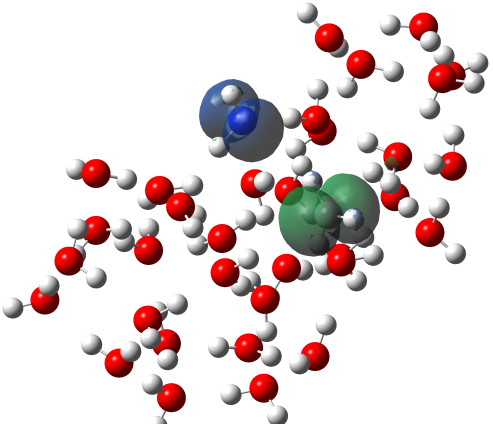
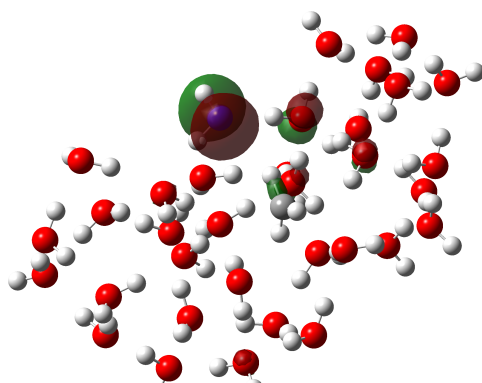
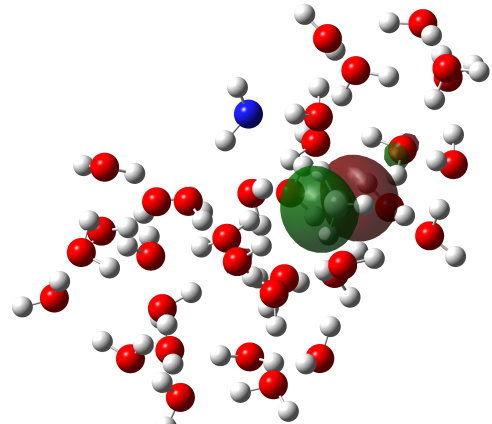
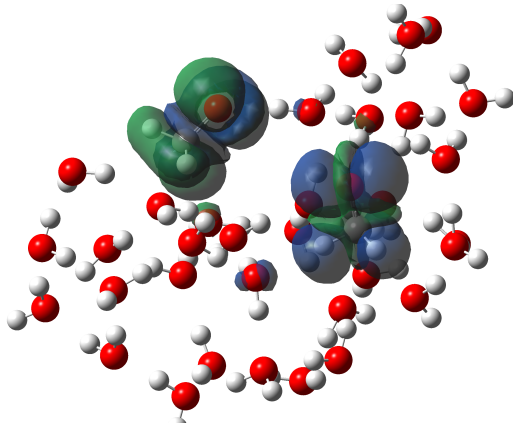
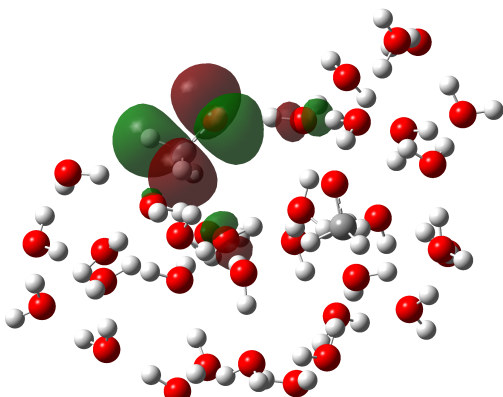
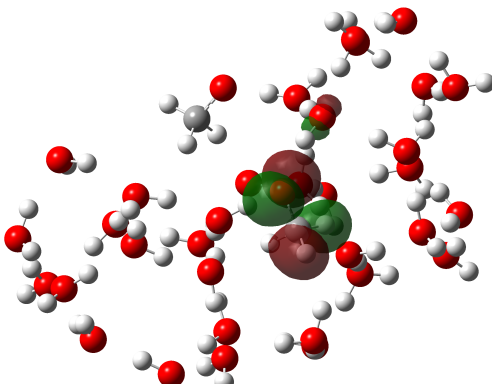
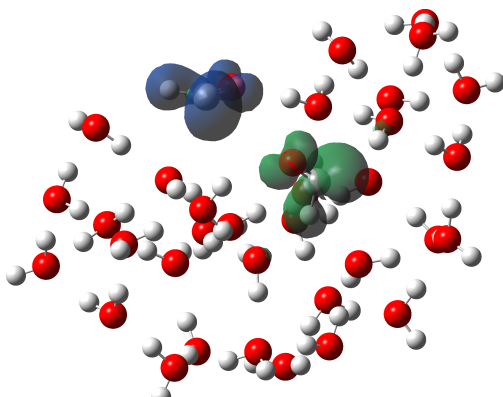
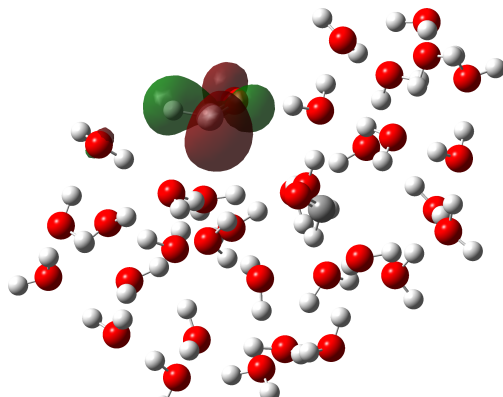
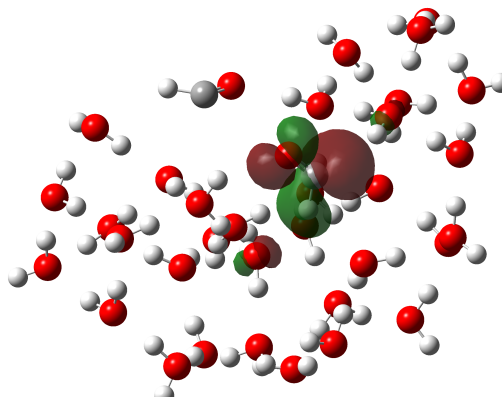
System	SD	α MO	β MO
CH₂OH + CH₂OH			
CH₃ + CH₂OH			
CH₃ + CH₃			
CH₃ + CH₃O		 HOMO-1	

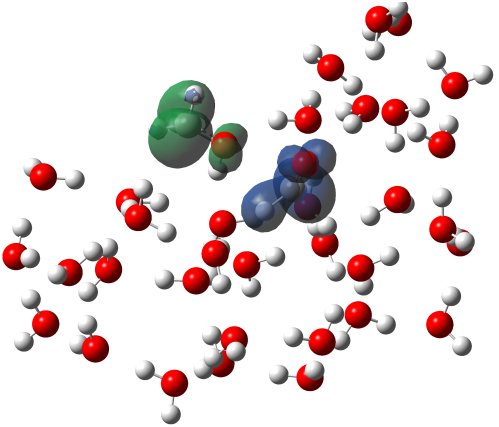
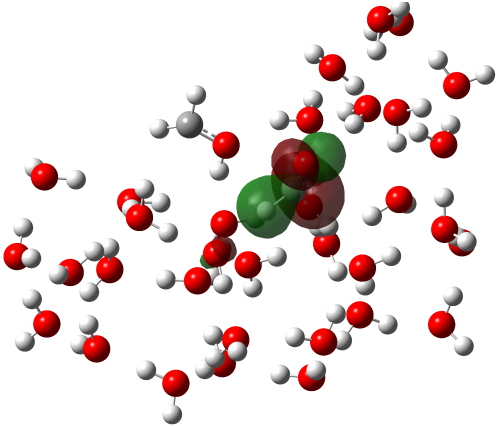
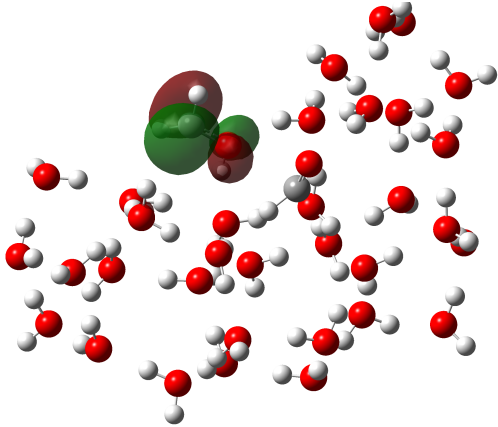
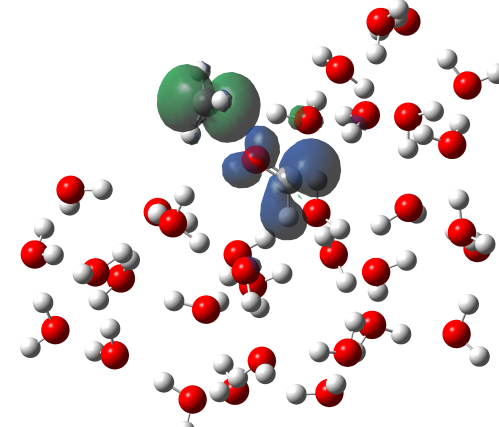
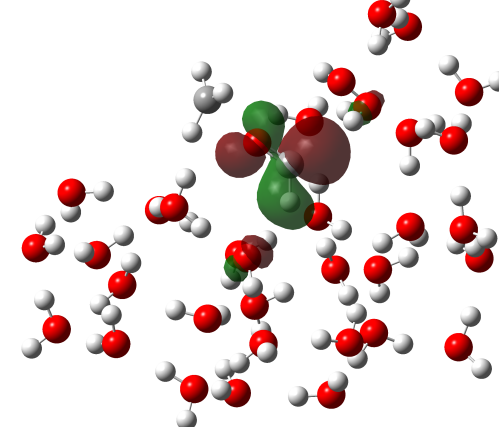
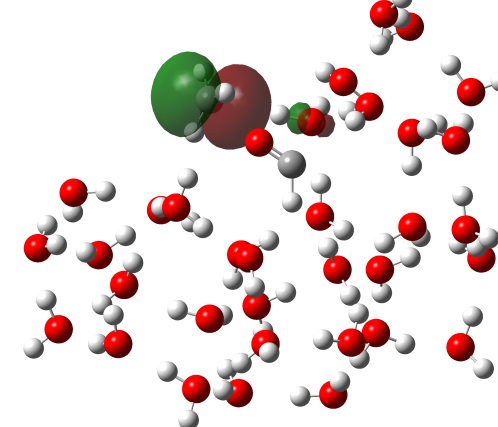
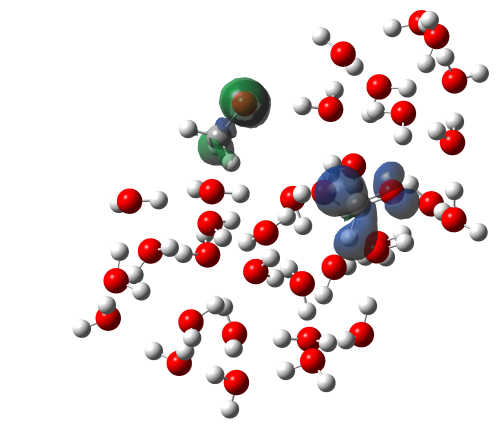
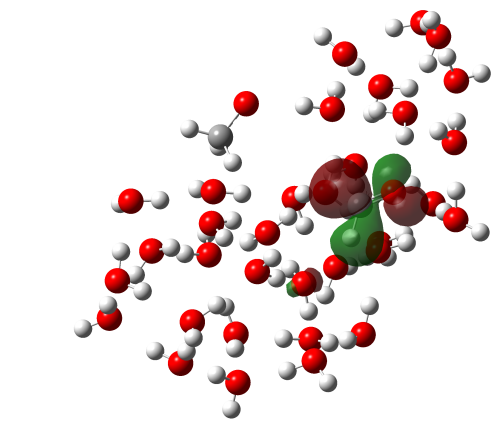
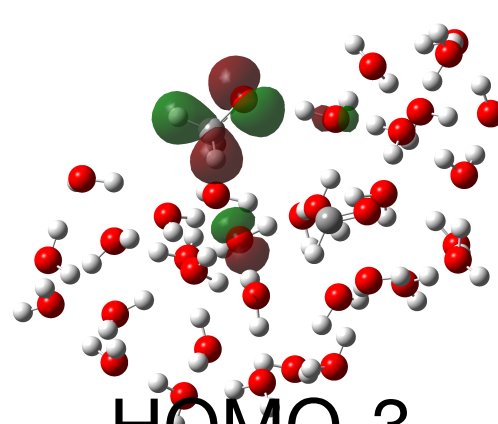
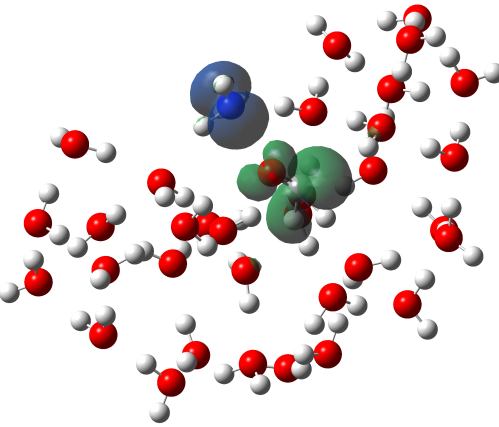
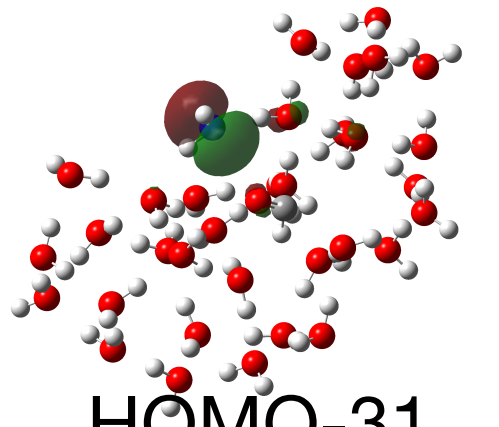
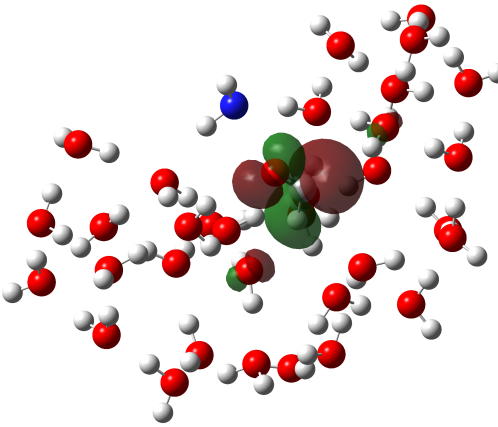
System	SD	α MO	β MO
CH ₃ + NH ₂			 HOMO-12
CH ₃ O + CH ₃ O			
HCO + HCO			
HCO + CH ₂ OH			

System	SD	α MO	β MO
CH ₃ + HCO			
HCO + CH ₃ O		 HOMO-3	
HCO + NH ₂		 HOMO-8	

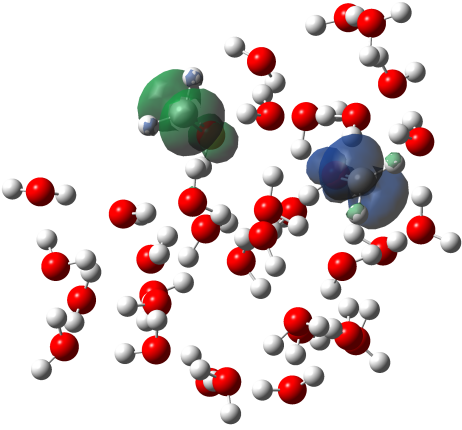
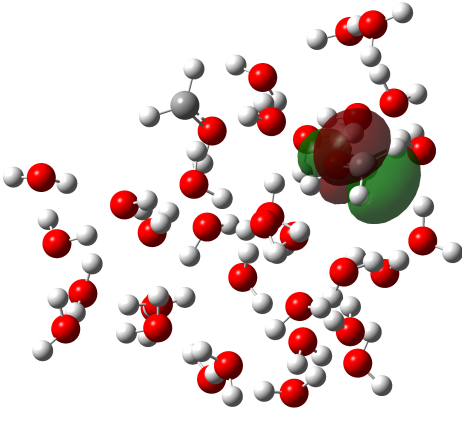
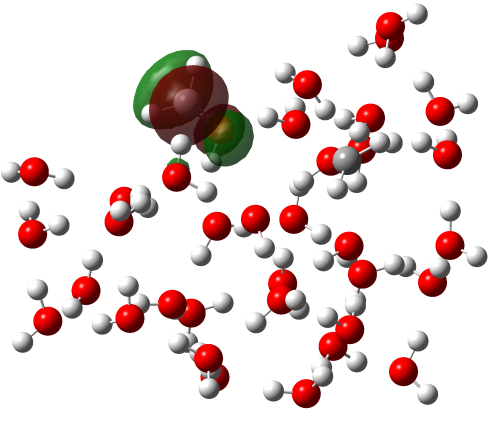
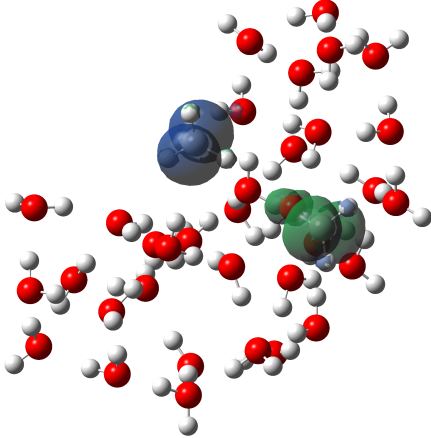
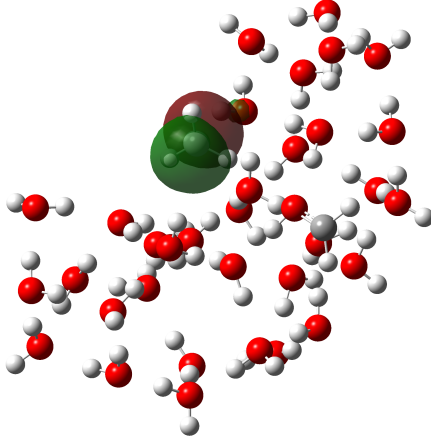
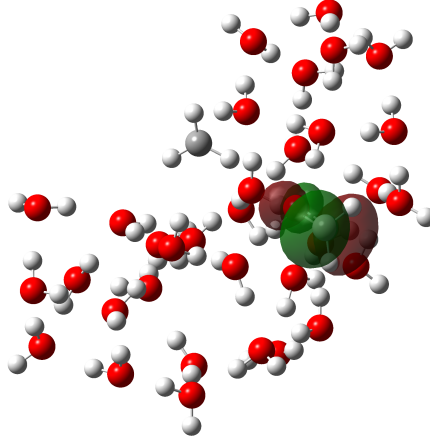
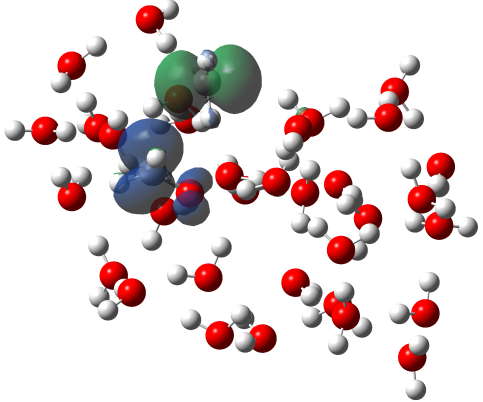
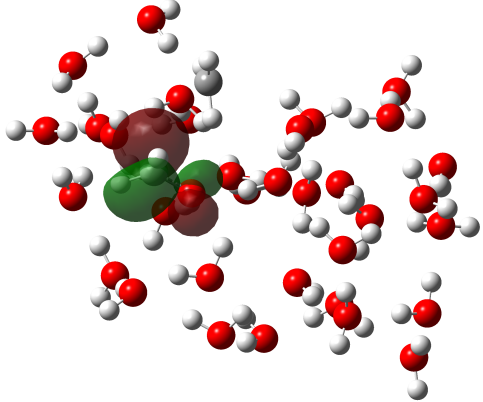
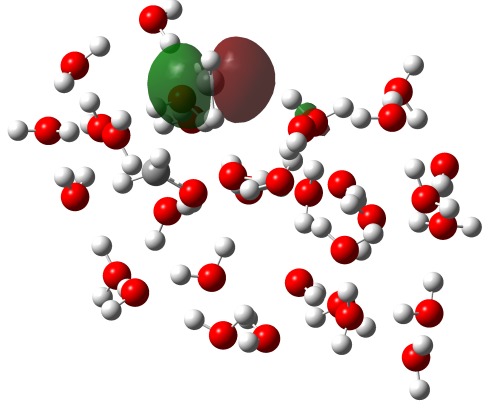
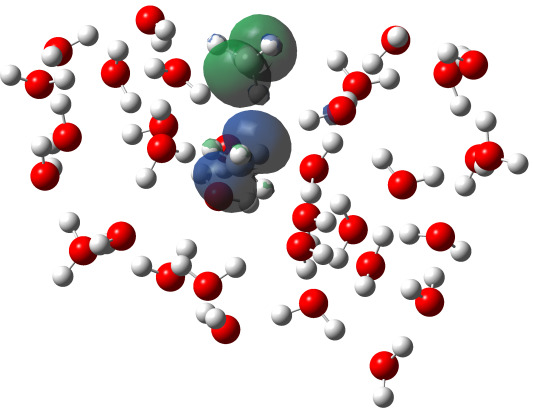
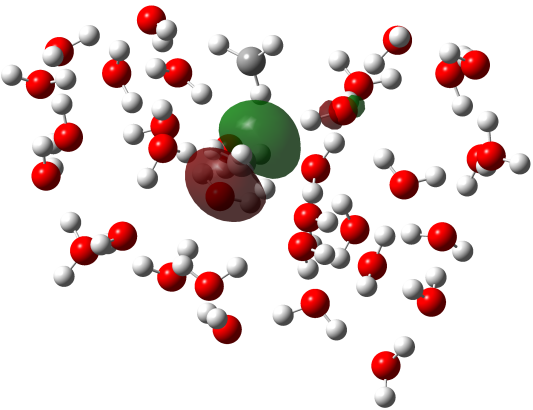
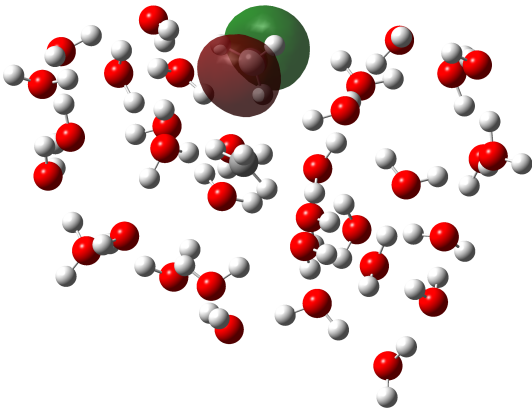
Reactants on W33

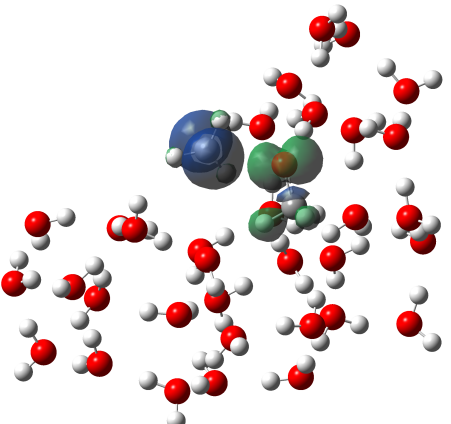
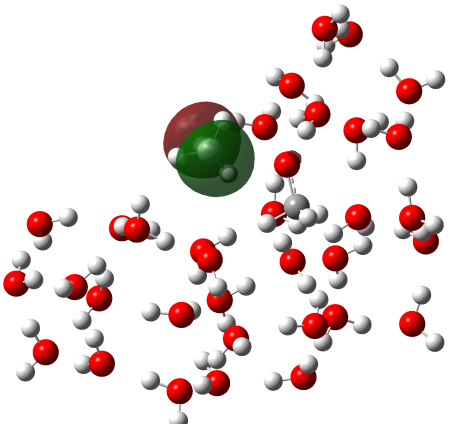
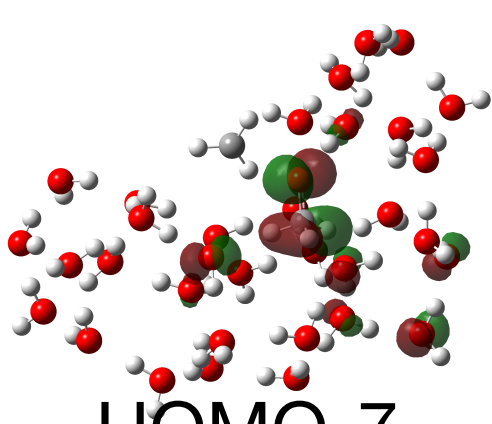
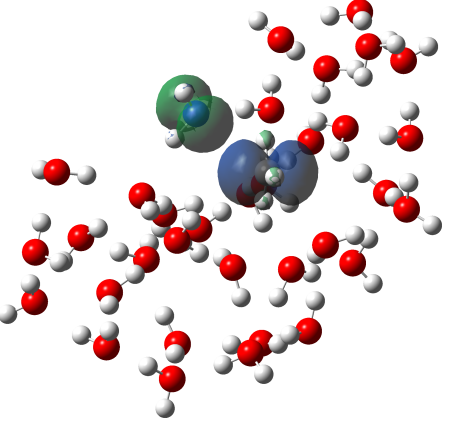
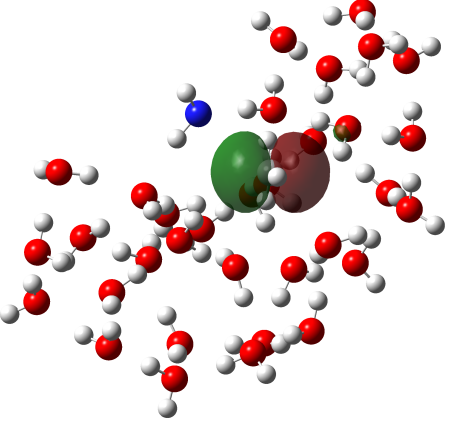
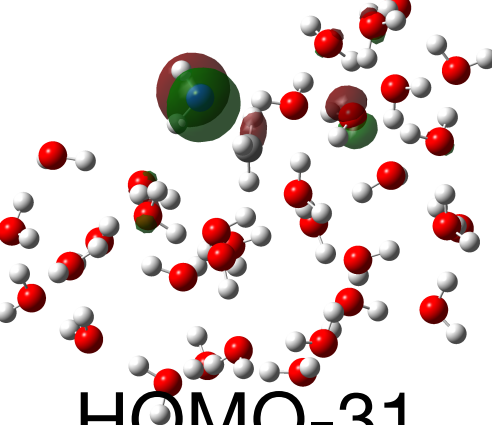
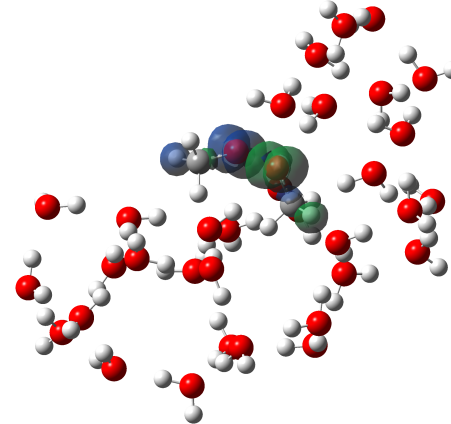
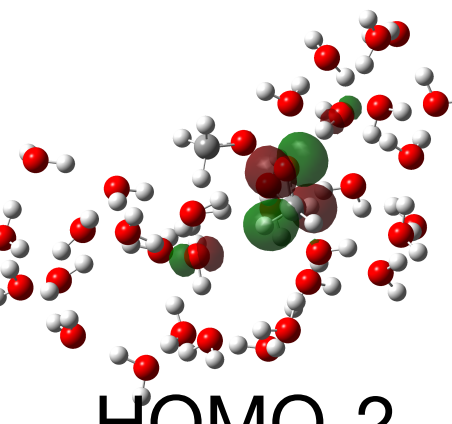
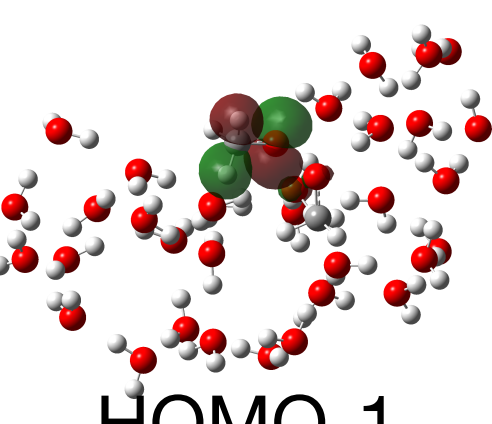
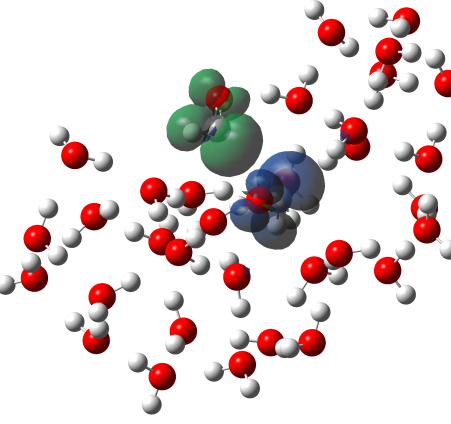
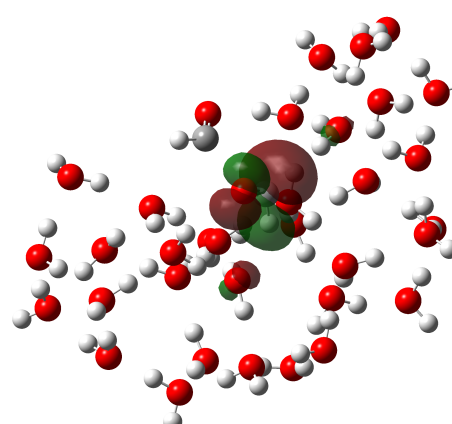
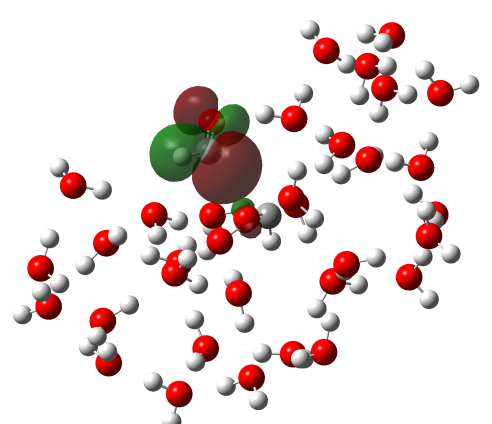
System	SD	α MO	β MO
CH ₂ OH + CH ₂ OH			
CH ₃ + CH ₂ OH STEP 1			
CH ₃ + CH ₂ OH STEP 2			
CH ₃ + CH ₃			

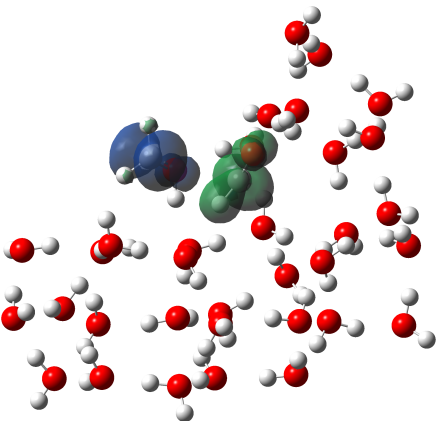
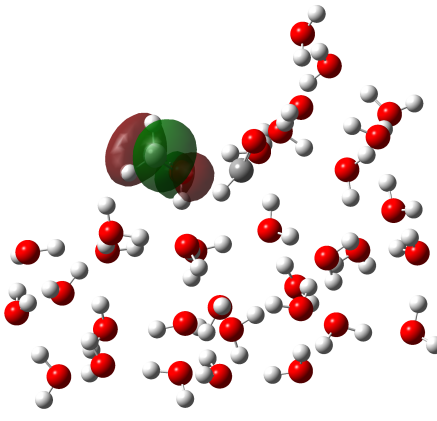
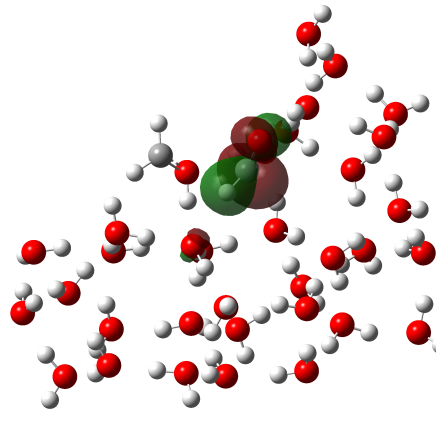
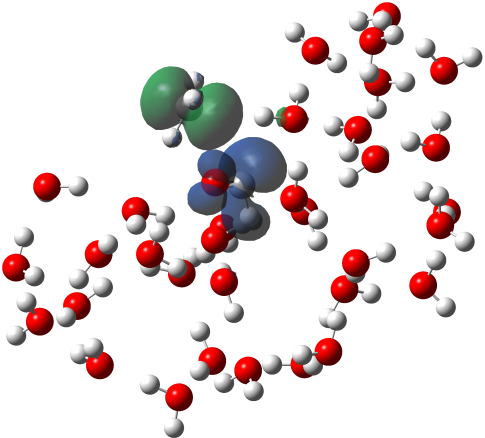
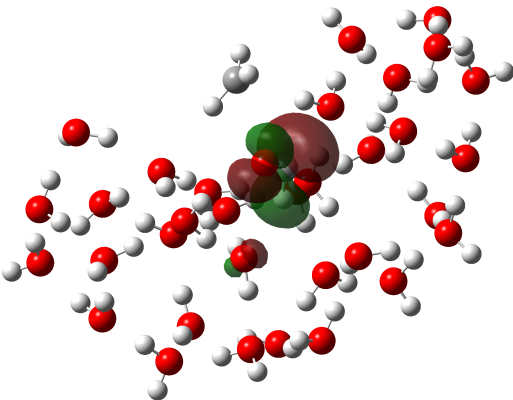
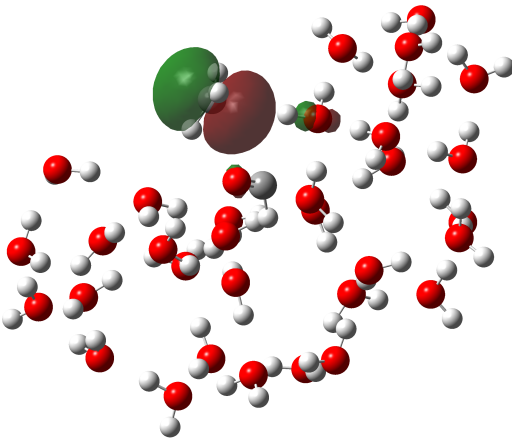
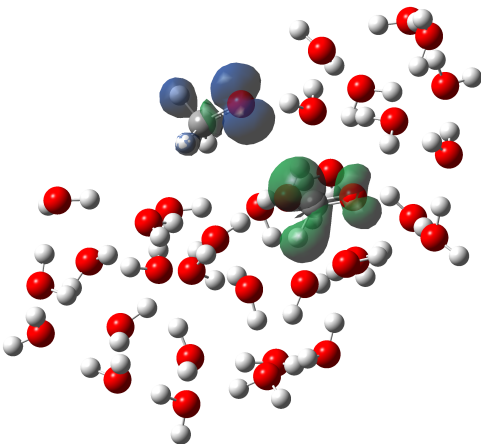
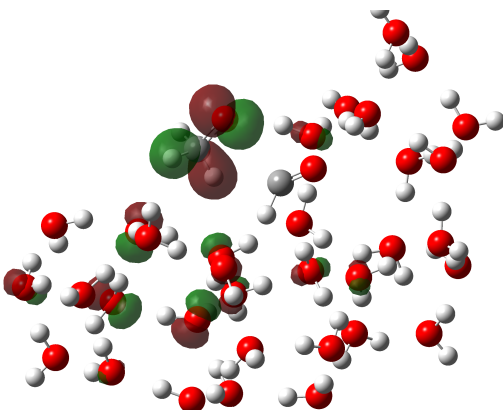
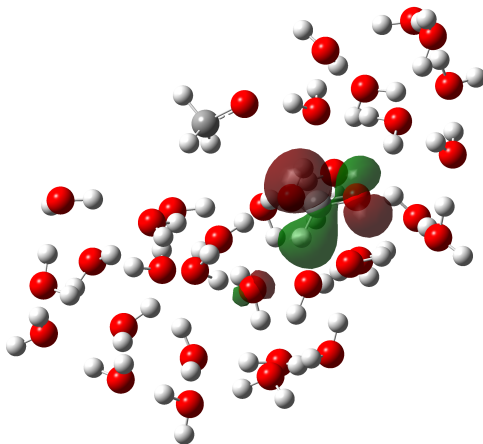
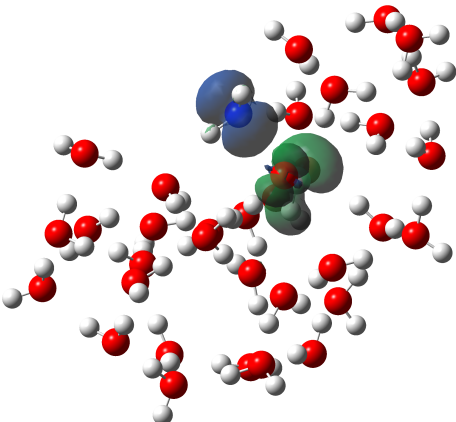
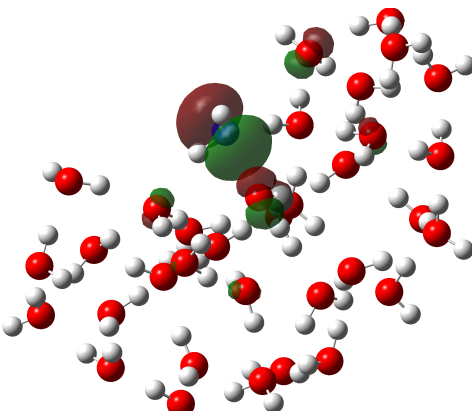
System	SD	α MO	β MO
CH₃ + CH₃O		 HOMO-7	
CH₃ + NH₂		 HOMO-33	
CH₃O + CH₃O		 HOMO-1	 HOMO-1
HCO + HCO			

System	SD	α MO	β MO
HCO + CH ₂ OH			
CH ₃ + HCO			
HCO + CH ₃ O			 HOMO-3
HCO + NH ₂		 HOMO-31	

TS on W33

System	SD	α MO	β MO
CH ₂ OH + CH ₂ OH			
CH ₃ + CH ₂ OH STEP 1			
CH ₃ + CH ₂ OH STEP 2			
CH ₃ + CH ₃			

System	SD	α MO	β MO
CH ₃ + CH ₃ O			 HOMO-7
CH ₃ + NH ₂			 HOMO-31
CH ₃ O + CH ₃ O		 HOMO-2	 HOMO-1
HCO + HCO			

System	SD	α MO	β MO
HCO + CH ₂ OH			
CH ₃ + HCO			
HCO + CH ₃ O		 HOMO-13	
HCO + NH ₂		 HOMO-30	