Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

N-Derivative of Shannon Entropy Density as Response Function

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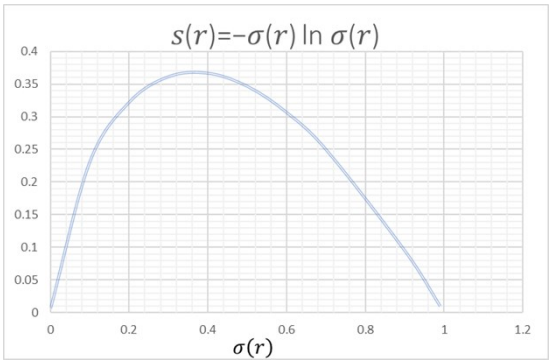


Fig. S1. Shannon entropy vs. shape function for CO molecule.

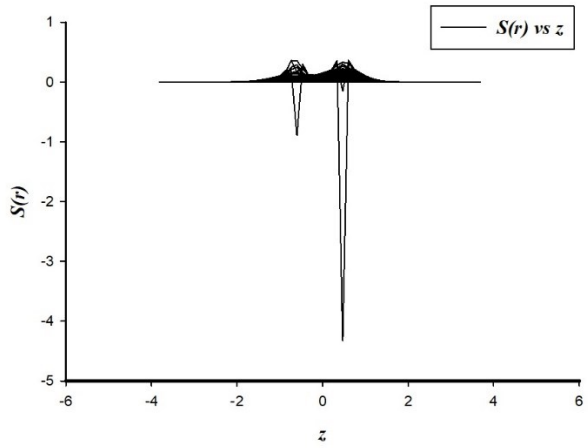


Fig. S2. Shannon entropy values along the C-O bond of carbon monoxide molecule.

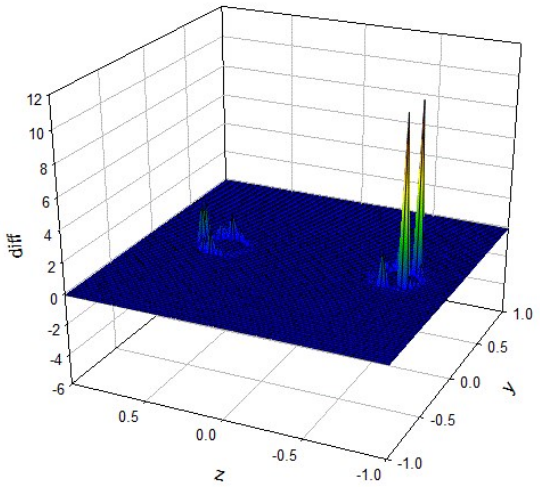
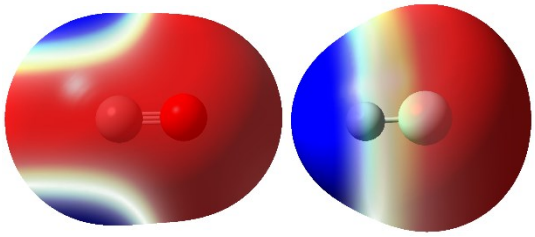
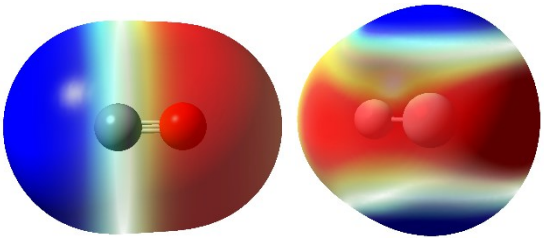


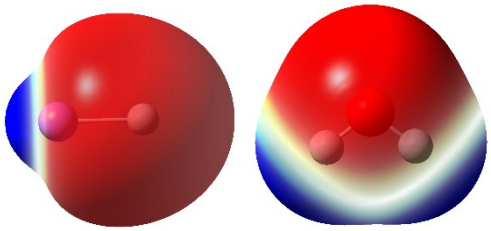
Fig. S3. Relative error of the approximate Shannon entropy density changes during the addition of an electron ($s^+(r)$) in CO molecular plane.



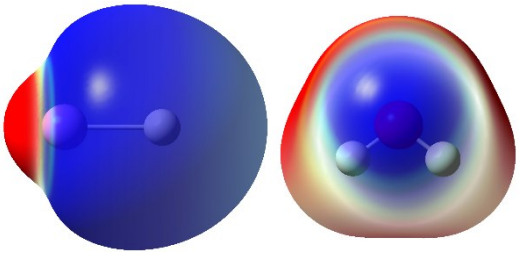
CO HF



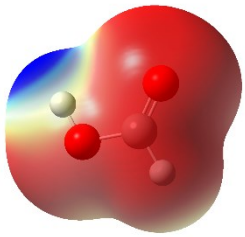
CO HF



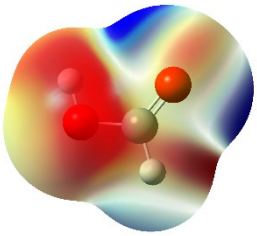
LiH H_2O



LiH H_2O



HCOOH



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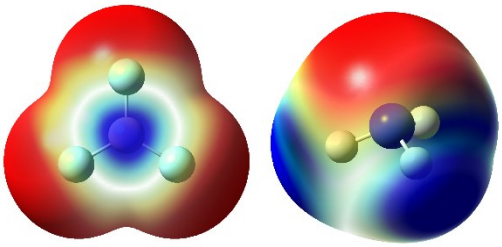
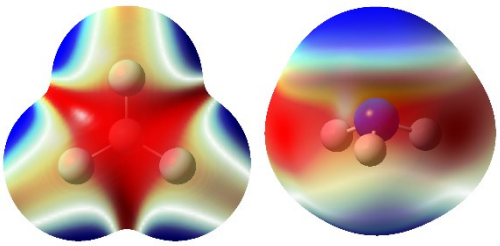


BF_3 NH_3



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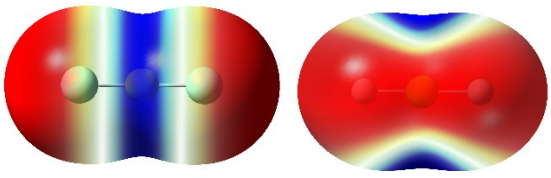
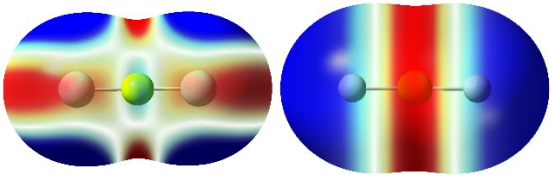
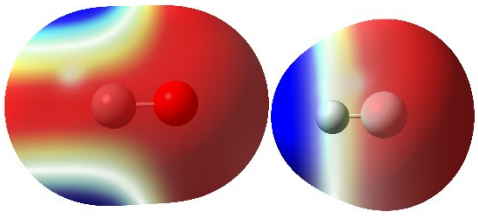


BeF_2 BeH_2

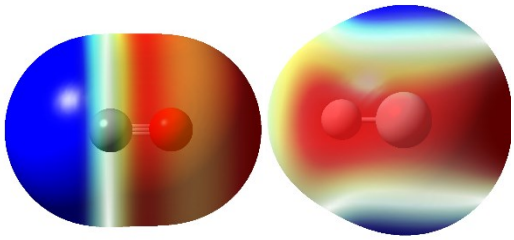


BeF_2 BeH_2

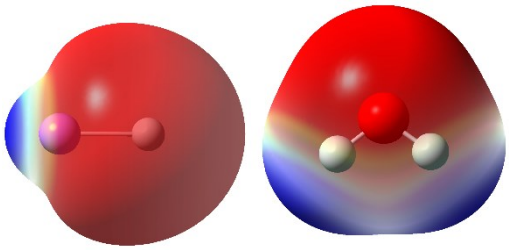
Fig. S4. Calculated $s^+(r)$ (left) and $s^-(r)$ (right) on the molecular surfaces of the considered molecules using B3LYP/6-311++G** method. The blue and red regions correspond to positive and negative values, respectively.



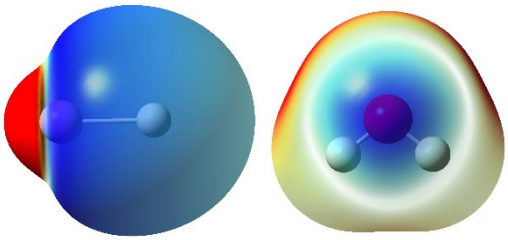
CO HF



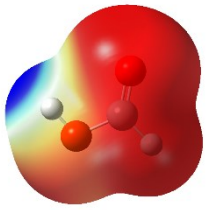
CO HF



LiH H_2O



LiH H_2O



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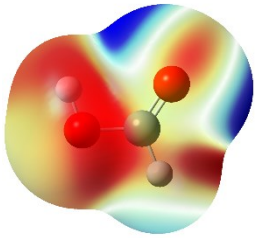
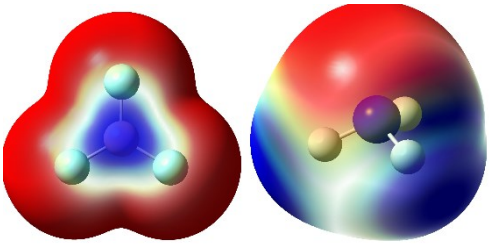
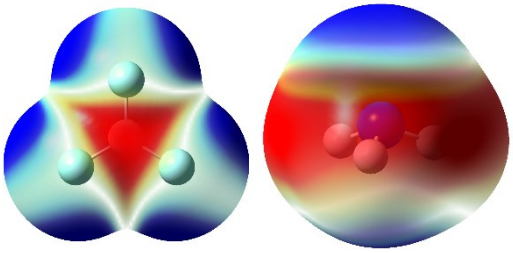


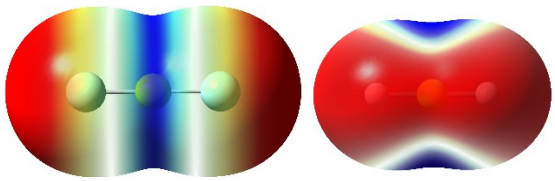
HCOOH



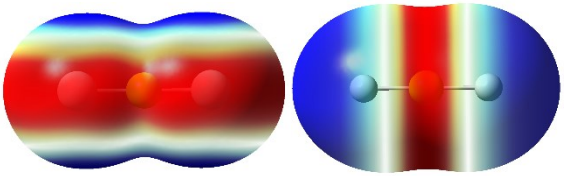
BF_3 NH_3



BF_3 NH_3

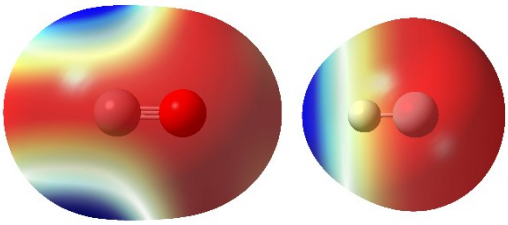


BeF_2 BeH_2

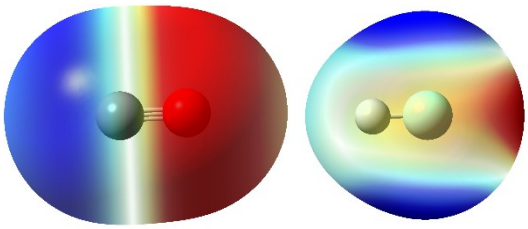


BeF_2 BeH_2

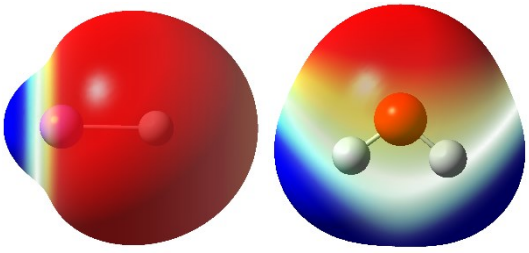
Fig. S5. Calculated $s^+(r)$ (left) and $s^-(r)$ (right) on the molecular surfaces of the considered molecules using MP2/6-311++G** method. The blue and red regions correspond to positive and negative values, respectively.



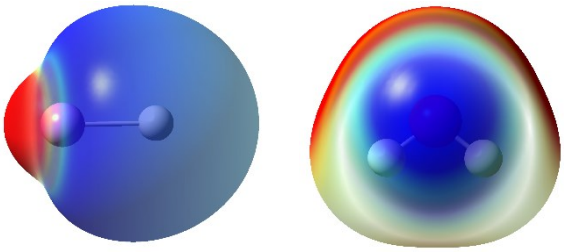
CO HF



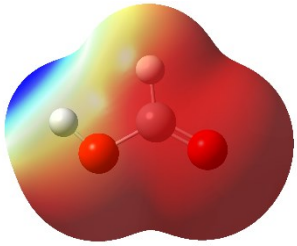
CO HF



LiH H_2O



LiH H_2O



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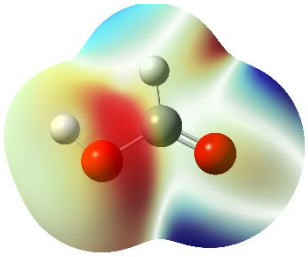

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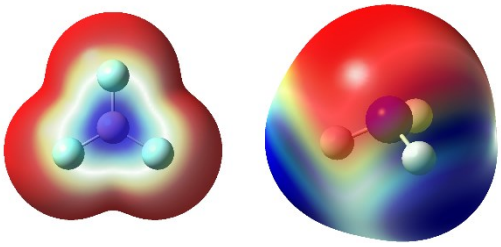
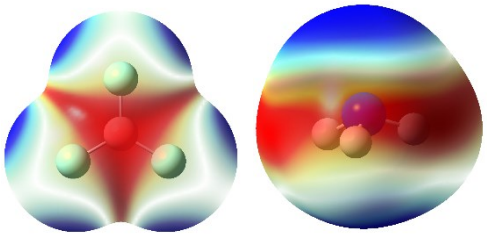
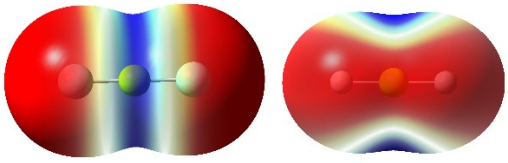


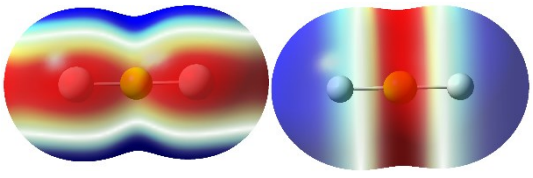
BF_3 NH_3



BF_3 NH_3



BeF_2 BeH_2



BeF_2 BeH_2

Fig. S6. Calculated $s^+(r)$ (left) and $s^-(r)$ (right) on the molecular surfaces of the considered molecules using MP2/aug-cc-pVTZ method. The blue and red regions correspond to positive and negative values, respectively.

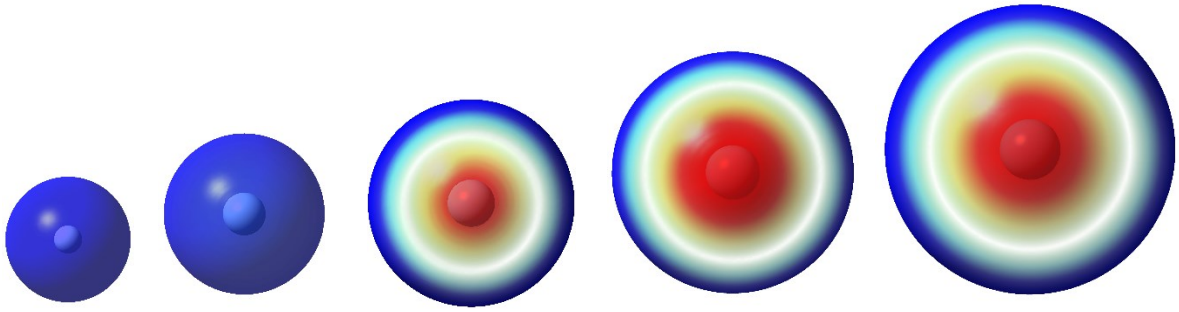


Fig. S7 Calculated dual Shannon entropy, $\Delta s(r)$, on the molecular surfaces of the noble gas atoms using M06/6-311++G** method. The blue and red regions correspond to positive and negative values, respectively.

Two density functional, which are defined as new user function for Multiwfn program, are as follow:

For first derivative $\frac{1+\ln\sigma(r)}{N}$ term:

userfunction=(1/nelec)*(1+log(fdens(x,y,z)/nelec))

For second derivative $\frac{1+ln\sigma(r)}{N^2}$ term:

userfunction=(1/nelec**2)*(1+log(fdens(x,y,z)/nelec))

The other .cub terms, such as Fukui function and shape function, are calculated using the pre-defined functions in Multiwfn program.