Electronic Supplementary Information

N-Derivative of Shannon Entropy Density as Response Function

Abdolkarim Matrodi and Siamak Noorizadeh*

Chemistry Department, Faculty of Sciences, Shahid Chamran University of Ahvaz, Ahvaz, Iran
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.
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.
**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.
**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 Multiwfnn program, are as follow:

\[
\frac{1 + \ln \sigma(r)}{N}
\]

For first derivative \(N\) term:

\[
\text{userfunction}=\frac{1}{\text{nelec}} \times (1 + \log(\text{fdens}(x,y,z) / \text{nelec}))
\]

\[
\frac{1 + \ln \sigma(r)}{N^2}
\]

For second derivative \(N^2\) term:

\[
\text{userfunction}=\frac{1}{\text{nelec}^2} \times (1 + \log(\text{fdens}(x,y,z) / \text{nelec}))
\]

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