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Shannon Informational Entropies and Chemical Reactivity

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1. Introduction

During the last decade, researchers around the world have shown that Information Theory [7] is probably one of the most important models in modern science. This model has given rise to applications and reinterpretations of concepts in Physics, Chemistry, Biology, Mathematics, Telecommunications and many other areas that are not, in principle, related to Information Theory. In the 90's, E. R. Frieden showed that important results such as the Schrödinger equation, the Maxwell-Boltzmann and Boltzmann distributions, the Dirac equation can be derived from principles of Information Theory [1–5].

Indded, information is a general concept that is perfectly applicable to any case. It is possible to ask what is the importance of the concept of information measure in quantum mechanics? What do they have in common the codes used to send messages from a communications' satellite have in common with the bases in a DNA molecule? How does the second law of Thermodynamics relate to Communication, to the extent that it is possible to speak of the entropy of a musical theme? How do the intricate problems of probability relate to the way we express ourselves orally or in writing? The answer to these questions can be found in *information*, and the fact that this concept can link very different ideas reveals its great generality and power.

In Chemistry, Information Theory has been applied to the characterization of chemical systems and chemical processes [10–13]. It has been shown that it is possible to use informational entropies to characterize processes such as bond breaking and bond formation. Shannon's entropy can be regarded as a general measure of information that can be used to obtain the Fukui function, which is a parameter of chemical reactivity in atomic and simple molecular systems [6]. In practice, the formal development of applications of Shannon's entropies in Density Functional Theory (DFT) is a fertile area of research. In this context the

maximum entropy method has been applied to DFT [33]. Following this line of research, we have initiated a new investigation to derive formal relationships between Information Theory concepts and Theoretical Chemistry.

In this work, we consider the idea that Shannon's entropy can be directly related to some fundamental DFT concepts. To show this, we present some simple mathematical derivations to prove that the first derivative of the Shannon entropy is directly related to DFT reactivity parameters such as the Fukui function, the hardness, softness, and chemical potential and that it might even be possible to obtain a formal relationship between Shannon's entropy and the electron energy. Finally, chemical applications are presented in which the relationships obtained in this work are used in two case studies involving a simple chemical reaction and a conformational analysis.

2. The first derivatives of Shannon's entropy and their relationship to chemical reactivity

For purposes of this chapter we take as a starting point the definition of the unnormalized Shannon's entropy in terms of the electron density in position space, which is defined as:

$$s(\mathbf{r}) = -\int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r}, \tag{1}$$

If normalized electron densities are used, $\frac{\rho(\mathbf{r})}{N}$, Shannon's entropy becomes positive: $S(\mathbf{r}) \geq 0$ and the normalized Shannon entropy is

$$S(\mathbf{r}) = -\int \frac{\rho(\mathbf{r})}{N} \ln \frac{\rho(\mathbf{r})}{N} d\mathbf{r}, \tag{2}$$

where N is the number of electrons. This expression can be rewritten as:

$$
\begin{aligned}
S(\mathbf{r}) &= -\frac{1}{N} \int \rho(\mathbf{r}) \ln \left(\frac{\rho(\mathbf{r})}{N} \right) d\mathbf{r} \\
&= -\frac{1}{N} \int \rho(\mathbf{r}) \left[\ln \rho(\mathbf{r}) - \ln N \right] d\mathbf{r} \\
&= -\frac{1}{N} \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{N} \ln N \underbrace{\int \rho(\mathbf{r}) d\mathbf{r}}_{=N} \\
&= -\frac{1}{N} \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} + \ln N \\
&= -\frac{s(\mathbf{r})}{N} + \ln N.
\end{aligned}
\tag{3}
$$

Differentiating the entropy $S(\mathbf{r})$ with respect to N at constant external potential $v(\mathbf{r})$:

$$\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} = -\frac{s(\mathbf{r})}{N^2} - \frac{1}{N}\int\left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{N}, \tag{4}$$

The term $\left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}$, is the Fukui function, which is a chemical reactivity parameter in DFT [33].

Also, we can set up the follow relationship

$$\left(\frac{\partial \rho(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})} = \left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})}, \tag{5}$$

and obtain the variation of Shannon's entropy with respect to the chemical potential:

$$\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} = -\frac{s(\mathbf{r})}{N^2}\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} - \frac{1}{N}\int\left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})}\ln\rho(\mathbf{r})d\mathbf{r}$$
$$+\frac{1}{N}\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} \tag{6}$$

simplify,

$$\left(\frac{\partial S(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})} = \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right]\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} - \frac{1}{N}\int\left(\frac{\partial \rho(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})}\ln\rho(\mathbf{r})d\mathbf{r}, \tag{7}$$

In this expression, we recognize the term $\left(\frac{\partial \rho(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})}$ which is the local softness.

Also, is it interesting to obtain the variation of Shannon's entropy with respect to the electron density,

$$\left(\frac{\partial S(\mathbf{r})}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} = -\frac{1}{N}\int 1 + \ln\rho(\mathbf{r})d\mathbf{r}. \tag{8}$$

A similar procedure can be used to obtain the above relations in momentum space as well as for the total Shannon entropy [14], which is defined as

$$S_T = S(\mathbf{r}) + S(\mathbf{p}), \tag{9}$$

where $S(\mathbf{r})$ and $S(\mathbf{p})$ are Shannon's entropies in position and momentum spaces, respectively. The variation of the total Shannon entropy with respect to electron number would be:

$$\frac{dS_T}{dN} = \left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} + \left(\frac{\partial S(\mathbf{p})}{\partial N}\right)_{v(\mathbf{p})}, \tag{10}$$

this permit us, open a door, to the study of this kind of derivatives and chemical descriptors, in momentum space. Results about, the chemical reactivity parameters in momentum space, will be present in other work.

Summarizing, the relations obtained are:

i)

$$\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} = -\frac{s(\mathbf{r})}{N^2} - \frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{N}. \tag{11}$$

ii)

$$\left(\frac{\partial S(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})} = \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right] \left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} - \frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r}. \tag{12}$$

iii)

$$\left(\frac{\partial S(\mathbf{r})}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} = -\frac{1}{N} \int 1 + \ln \rho(\mathbf{r}) d\mathbf{r}. \tag{13}$$

In the formalism of DFT, the reactivity parameters are defined as:

$$\text{Chemical potential} = \mu = \left(\frac{\partial E}{\partial N}\right)_{v(\mathbf{r})}. \tag{14}$$

$$\text{Hardness} = \eta = \left(\frac{\partial \mu}{\partial N}\right)_{v(\mathbf{r})} = \left(\frac{\partial^2 E}{\partial N^2}\right)_{v(\mathbf{r})}. \tag{15}$$

$$\text{Softness} = s = \left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})} = \left(\frac{\partial \rho(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})}. \tag{16}$$

$$\text{Fukui function} = f(\mathbf{r}) = \left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}. \tag{17}$$

where μ is the Chemical potential, η is the Hardness, s is the Softness and $f(\mathbf{r})$ is the Fukui Function. Each one of these equations has a specific interpretation in Chemistry. The Chemical potential, μ, is a measure the escaping tendency of an electron, which is constant, through all space, for the ground state of an atom, molecule, or solid [16]. The Hardness, η, is related to the polarizability [15] and the Fukui function [23–25], $\left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}$, is interpreted as a measure of the sensitivity of the chemical potential with respect to an external perturbation at a particular point. These properties have been included in the chemical vocabulary since the early 1950s.

2.1. The second derivatives of Shannon's entropy

In this section we obtain the second derivatives of the Shannon entropy respect to the electron density, how a first case, we take the Eq. (11),

$$
\begin{aligned}
\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r}) \partial N} \right)_{v(\mathbf{r})} &= \frac{\partial}{\partial \rho(\mathbf{r})} \left\{ -\frac{s(\mathbf{r})}{N^2} - \frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial N} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{N} \right\} \\
&= -\frac{1}{N^2} \int 1 + \ln \rho(\mathbf{r}) d\mathbf{r} \\
&\quad - \frac{1}{N} \int \left(\frac{\partial f(\mathbf{r})}{\partial \rho(\mathbf{r})} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) + \frac{f(\mathbf{r})}{\rho(\mathbf{r})} d\mathbf{r}.
\end{aligned}
\tag{18}
$$

where $f(\mathbf{r})$ is it the Fukui function.

How a second case, consider the Eq. (12),

$$
\begin{aligned}
\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r}) \partial \mu} \right)_{v(\mathbf{r})} &= \frac{\partial}{\partial \rho(\mathbf{r})} \left\{ \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2} \right] \left(\frac{\partial N}{\partial \mu} \right)_{v(\mathbf{r})} - \int \left(\frac{\partial \rho(\mathbf{r})}{\partial \mu} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} \right\} \\
&= -\frac{1}{N^2} \left(\frac{\partial N}{\partial \mu} \right)_{v(\mathbf{r})} \int 1 + \ln \rho(\mathbf{r}) d\mathbf{r} \\
&\quad - \int \left(\frac{\partial s}{\partial \rho(\mathbf{r})} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) + \frac{s}{\rho(\mathbf{r})} d\mathbf{r}.
\end{aligned}
\tag{19}
$$

where s is the softness.

Finally, for Eq. (13),

$$
\begin{aligned}
\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r})^2} \right)_{v(\mathbf{r})} &= -\frac{1}{N} \int \frac{\partial}{\partial \rho(\mathbf{r})} (1 + \ln \rho(\mathbf{r})) \, d\mathbf{r} \\
&= -\frac{1}{N} \int \frac{d\mathbf{r}}{\rho(\mathbf{r})}.
\end{aligned}
\tag{20}
$$

2.2. The change of Shannon entropy respect to the electron energy using Parr-Gadre-Bartolotti model

Now, we obtain the variation of the Shannon entropy respect to the energy, in this case, consider the chemical potential $\mu = \left(\frac{\partial E}{\partial N} \right)_{v(\mathbf{r})}$ and the Eq. (4),

$$
\begin{aligned}
\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})} &= -\frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} \\
&\quad + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right] \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})} \\
&= -\frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial E}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} \\
&\quad + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right] \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})},
\end{aligned}
\tag{21}
$$

note the importance of this relation, we can establish a formal relation between the Shannon entropy with the electronic energy[1].

In a similar way, we can obtain the second derivative of the last equation respect to electron density.

$$
\begin{aligned}
\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r}) \partial E}\right)_{v(\mathbf{r})} &= \frac{\partial}{\partial \rho(\mathbf{r})} \left\{ -\frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial E}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right] \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})} \right\} \\
&= -\frac{1}{N} \int \left(\frac{\partial \mu(\mathbf{r})}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) + \frac{\mu(\mathbf{r})}{\rho(\mathbf{r})} d\mathbf{r} \\
&\quad - \frac{1}{N^2} \left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})} \int 1 + \ln \rho(\mathbf{r}) d\mathbf{r}.
\end{aligned}
\tag{22}
$$

where $\mu(\mathbf{r})$ it is a local chemical potential.

For obtain a direct application of the last result in the DFT model, we selected the Parr-Gadre-Bartolotti model [26], PGB, this is a local model based in the Thomas-Fermi model [17, 18]. The expression for the energy in the PGB model is,

$$
d \left[E\right]_{PGB} = C\rho(\mathbf{r})^{5/3} + \rho(\mathbf{r})v(\mathbf{r}) + BN^{2/3}\rho(\mathbf{r})^{4/3} d\mathbf{r},
\tag{23}
$$

where $B = 0.7544$ and $C = 3.8738$.

Considering Eq. (21), and Eq. (23), the first step is it obtain $\left(\frac{\partial \rho(\mathbf{r})}{\partial E}\right)_{v(\mathbf{r})}$, for do this, consider

$$
\left(\frac{\partial \rho(\mathbf{r})}{\partial E_{PGB}}\right)_{v(\mathbf{r})}^{-1} = \left(\frac{\partial E_{PGB}}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})}
\tag{24}
$$

---

[1] A more complete study about of the formal relation between electron energy and Shannon entropy will present in other work.

with this and the Eq. (23),

$$\left(\frac{\partial E_{PGB}}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} = \frac{\partial}{\partial \rho(\mathbf{r})}\left\{C\rho(\mathbf{r})^{5/3} + \rho(\mathbf{r})v(\mathbf{r}) + BN^{2/3}\rho(\mathbf{r})^{4/3}\right\}$$

$$= \frac{5}{3}C\rho(\mathbf{r})^{2/3} + v(\mathbf{r}) + \frac{4}{3}BN^{2/3}\rho(\mathbf{r})^{1/3} \tag{25}$$

and,

$$\left(\frac{\partial \rho(\mathbf{r})}{\partial E_{PGB}}\right)_{v(\mathbf{r})} = \frac{1}{\frac{5}{3}C\rho(\mathbf{r})^{2/3} + v(\mathbf{r}) + \frac{4}{3}BN^{2/3}\rho(\mathbf{r})^{1/3}}, \tag{26}$$

now consider the Eq. (21),

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_{PGB}}\right)_{v(\mathbf{r})} = -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\frac{5}{3}C\rho(\mathbf{r})^{2/3} + v(\mathbf{r}) + \frac{4}{3}BN^{2/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r} + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right]\left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})}. \tag{27}$$

The importance of this results, resides in that for the first time we prove that there exist a formal relationship between concepts of the information theory and the chemical reactivity, based on a formal derivation rather than on a phenomenological interpretation.

2.3. The variation of Shannon's entropy with respect to the electron kinetic energy

In this case, we consider the famous Thomas-Fermi kinetic energy functional, defined as

$$dE_k^{TF}[\rho(\mathbf{r})] = C_F\rho(\mathbf{r})^{5/3}d\mathbf{r}, \qquad C_F = \frac{3}{10}(3\pi^2)^{2/3}, \tag{28}$$

first we use the property (24)

$$\left(\frac{\partial E_k^{TF}}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} = C_F\frac{5}{3}\rho(\mathbf{r})^{2/3}, \tag{29}$$

now, we use the Eq. (21)

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_k^{TF}}\right)_{v(\mathbf{r})} = -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{C_F\frac{5}{3}\rho(\mathbf{r})^{2/3}}d\mathbf{r} + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right]\frac{1}{\mu},$$

$$= -\frac{3}{5NC_F}\int \frac{\ln\rho(\mathbf{r})}{\rho(\mathbf{r})^{2/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}. \tag{30}$$

2.4. The variation of Shannon's entropy with respect to the exchange energy in LDA

For simplicity we take only the exchange energy, in the Local Density Approximation (LDA), in this approximation the total energy of a system can be write as the sum of the correlation and exchange energy: $\varepsilon_{cx} = \varepsilon_x + \varepsilon_c$. The correlation part, ε_c has been calculated and the results obtained were expressed like complicated expression of $\rho(\mathbf{r})$ [27]. In our case, we only consider the exchange term, defined as

$$dE_x^{LDA}[\rho(\mathbf{r})] = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{4/3}d\mathbf{r} \tag{31}$$

again,

$$\left(\frac{\partial E_x^{LDA}}{\partial \rho(\mathbf{r})}\right)_{v(\mathbf{r})} = -\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}, \tag{32}$$

and

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_x^{LDA}}\right)_{v(\mathbf{r})} = -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r} + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right]\left(\frac{\partial N}{\partial E}\right)_{v(\mathbf{r})}$$

$$= -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}. \tag{33}$$

2.5. Variation of Shannon's entropy with respect to the energy, considering the kinetic and exchange effects.

Now, we can take the previous results to obtain the variation on Shannon's entropy considering the kinetic and exchange effects using local models. This derivative will be

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_{k,x}^{TF,LDA}}\right)_{v(\mathbf{r})} = \left(\frac{\partial S(\mathbf{r})}{\partial E_k^{TF}}\right)_{v(\mathbf{r})} + \left(\frac{\partial S(\mathbf{r})}{\partial E_x^{LDA}}\right)_{v(\mathbf{r})}$$

$$= -\frac{3}{5NC_F}\int \frac{\ln\rho(\mathbf{r})}{\rho(\mathbf{r})^{2/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}$$

$$- \frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}$$

$$= \left[-\frac{3}{5NC_F}\int \frac{\ln\rho(\mathbf{r})}{\rho(\mathbf{r})^{2/3}}d\mathbf{r} - \frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r}\right]$$

$$- \frac{1}{\mu N^2} \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{\mu N}$$

$$= -\frac{1}{N} \left(\frac{3}{5C_F} + \frac{1}{(3/\pi)^{1/3}} \right) \int \left(\frac{1 + \rho(\mathbf{r})^{1/3}}{\rho(\mathbf{r})^{2/3}} \right) \ln \rho(\mathbf{r}) d\mathbf{r}$$

$$- \frac{1}{\mu N^2} \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{\mu N}$$

$$= -\int \left[A \left(\frac{1 + \rho(\mathbf{r})^{1/3}}{\rho(\mathbf{r})^{2/3}} \right) - B\rho(\mathbf{r}) \right] \ln \rho(\mathbf{r}) d\mathbf{r} + BN, \tag{34}$$

where

$$A = \frac{3}{5NC_F} + \frac{1}{N(3/\pi)^{2/3}},$$

and

$$B = \frac{1}{\mu N^2}.$$

2.6. Summary of relationships obtained

Finally, we present a summary of the different relations obtained in this work. Whit this results, is possible say that the information theory is a model that is subjacent to the Density Functional Theory.

In the follow section we show some results of this relations applied to some chemical process.

$$\left(\frac{\partial S(\mathbf{r})}{\partial N} \right)_{v(\mathbf{r})} = -\frac{s(\mathbf{r})}{N^2} - \frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial N} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} + \frac{1}{N}. \tag{35}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial \mu} \right)_{v(\mathbf{r})} = \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2} \right] \left(\frac{\partial N}{\partial \mu} \right)_{v(\mathbf{r})} - \frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial \mu} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r}. \tag{36}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial \rho(\mathbf{r})} \right)_{v(\mathbf{r})} = -\frac{1}{N} \int 1 + \ln \rho(\mathbf{r}) d\mathbf{r}. \tag{37}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial E} \right)_{v(\mathbf{r})} = -\frac{1}{N} \int \left(\frac{\partial \rho(\mathbf{r})}{\partial E} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) d\mathbf{r} + \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2} \right] \left(\frac{\partial N}{\partial E} \right)_{v(\mathbf{r})}. \tag{38}$$

$$\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r}) \partial N} \right)_{v(\mathbf{r})} = -\frac{1}{N} \int \left(\frac{\partial f(\mathbf{r})}{\partial \rho(\mathbf{r})} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) + \frac{f(\mathbf{r})}{\rho(\mathbf{r})} d\mathbf{r}. \tag{39}$$

$$\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r}) \partial \mu} \right)_{v(\mathbf{r})} = -\int \left(\frac{\partial s}{\partial \rho(\mathbf{r})} \right)_{v(\mathbf{r})} \ln \rho(\mathbf{r}) + \frac{s}{\rho(\mathbf{r})} d\mathbf{r}. \tag{40}$$

$$\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r})^2} \right)_{v(\mathbf{r})} = -\frac{1}{N} \int \frac{d\mathbf{r}}{\rho(\mathbf{r})}. \tag{41}$$

$$\left(\frac{\partial^2 S(\mathbf{r})}{\partial \rho(\mathbf{r})\partial E}\right)_{\nu(\mathbf{r})} = -\frac{1}{N^2}\left(\frac{\partial N}{\partial E}\right)_{\nu(\mathbf{r})}\int 1 + \ln\rho(\mathbf{r})d\mathbf{r}. \tag{42}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_k^{TF}}\right)_{\nu(\mathbf{r})} = -\frac{3}{5NC_F}\int \frac{\ln\rho(\mathbf{r})}{\rho(\mathbf{r})^{2/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}. \tag{43}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial E_x^{LDA}}\right)_{\nu(\mathbf{r})} = -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\left(\frac{3}{\pi}\right)^{1/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r} - \frac{1}{\mu N^2}\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} + \frac{1}{\mu N}. \tag{44}$$

$$\left(\frac{S(\mathbf{r})}{E_{k,x}^{TF,LDA}}\right)_{\nu(\mathbf{r})} = -\int \left[A\left(\frac{1+\rho(\mathbf{r})^{1/3}}{\rho(\mathbf{r})^{2/3}}\right) - B\rho(\mathbf{r})\right]\ln\rho(\mathbf{r})d\mathbf{r} + BN. \tag{45}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial E^{PGB}}\right)_{\nu(\mathbf{r})} = -\frac{1}{N}\int \frac{\ln\rho(\mathbf{r})}{\frac{5}{3}C\rho(\mathbf{r})^{2/3} + \nu(\mathbf{r}) + \frac{4}{3}BN^{2/3}\rho(\mathbf{r})^{1/3}}d\mathbf{r}$$
$$+ \left[\frac{1}{N} - \frac{s(\mathbf{r})}{N^2}\right]\left(\frac{\partial N}{\partial E}\right)_{\nu(\mathbf{r})}. \tag{46}$$

3. Description of a simple chemical process

3.1. Reaction $CH_2CHF + CH_3 \rightarrow CH_3CHFCH_2$

To show the application of the relations obtained, we have selected the following radical-molecule chemical reaction: $CH_2CHF + CH_3 \rightarrow CH_3CHFCH_2$.

Structures and energies have been obtained along the reaction path using m062x/6-311++G(d,p) density functional method with Gaussian 09 [31]. The electron density was calculated with Pérez-Jordá's algorithms [8] and a D-Grid 4.6 [9]. Molecular Electrostatic Potential (MEP) isosurfaces were obtained with Molden 5.0 [22]. The Fukui function condensed was calculated using natural atomics orbitals obtained in a Natural Population Analysis [28].

The condensed Fukui function were calculated according to the following approximations:

$$f(\mathbf{r})^+ = |\phi(\mathbf{r})_{\text{LUMO}}|^2 + \sum_{i=1}^{n}\frac{\partial}{\partial N}|\phi(\mathbf{r})|^2. \tag{47}$$

$$f(\mathbf{r})^- = |\phi(\mathbf{r})_{\text{HOMO}}|^2 + \sum_{i=1}^{n}\frac{\partial}{\partial N}|\phi(\mathbf{r})|^2. \tag{48}$$

$$f(\mathbf{r}) = \frac{1}{2}\left(f(\mathbf{r})^+ + f(\mathbf{r})^-\right). \tag{49}$$

where $\phi(\mathbf{r})_{\text{LUMO}}$ correspond to LUMO electron density and $\phi(\mathbf{r})_{\text{HOMO}}$ to HOMO electron density. When a molecule accepts electrons, the electrons tend to go to places where $f(\mathbf{r})^+$ is large because it is at these locations that the molecule is most able to stabilize additional electrons. Therefore a molecule is susceptible of a nucleophilic attack at sites where $f(\mathbf{r})^+$

is large. Similarly, a molecule is susceptible of an electrophilic attack at sites where $f(\mathbf{r})^-$ is large, because these are the regions where electron removal destabilizes the molecule the least. In chemical density functional theory, the Fukui functions are the key regioselectivity indicators for electron-transfer controlled reactions. In order to use these expressions we have chosen the Natural Population Analysis, NPA, which involves only matrix diagonalization of small subsets of the density matrix, and also requires a negligible amount of computer time. Although it is more involved than a Mulliken or Löwdin analysis, for a theoretical analysis using von Neumann entropies, NPA is an attractive method [29, 30, 34].

In Figure (1(a)) we present the electron energy profile of the reaction as a function of the reaction coordinate RX in Å. Trends in the condensed Fukui function are shown in Figure (1(b)). Analogously, trends in Hardness and chemical potential are shown in Figures (1(c)) and (1(d)), respectively.

In Figures (2(a)) and (2(b)) we present the trends in the kinetic and exchange energies as a function of the reaction coordinate.

Energy values show that the reaction is exothermic, with the following energy values at stationary points: E(reactants)=-217.629652 A.U.; E(transition state)= -217.615808 A.U. and E(products)= -217.674564 A.U. One of the main points of interest for our purposes is the analysis of the structures along the reaction path in terms of descriptors that are related to chemical reactivity. In this specific case, we consider the kinetic and exchange energies (see Figs. (2(a)) and (2(b))). For the kinetic energy we note that there exists a region limited by a maximum at $RX = -0.64230$ and a minimum at $RX = 1.44550$, in which important chemical changes occurs. It is associated with bond forming, in the Figures (2(c))-(2(l)) present the Molecular Electrostatic Potential of this process, probably this result permit us establish a kinetically classification criteria of this reaction, that is, the principal parameter that govern this process it is the kinetic. The minima in $RX = 1.44550$ is it in relation to important chemical changes that occurs in the frontier orbitals, see the Figures (2(m)), (2(n)) (2(o)) and (2(p)) where present the isosurfaces of the HOMO and LUMO orbitals.

In the case of the Hardness, we note that not are a correspondence between the maximum or minima of the electron, kinetic or exchange energy with the minimum and maximum of the Hardness. This points, again are related at with the structural changes that occurs in this zone, also, of course, this changes involved important changes in the frontier orbitals. A similar aspect occurs with the condensed Fukui functions, Figure (1(b)), where we note that in the point $RX = 0.32119$ exist a equality $f(\mathbf{r})^+ \simeq f(\mathbf{r})^- \simeq f(\mathbf{r}) \simeq 0.5$ with this numerical result we can note a parallelism with the relation of a hard/soft acids/basis, proposed by Pearson. That in terms of the condensed Fukui functions would be, when a chemical process occurs, exist a point where the active sites of the structures have a equalization of a kind of chemical attack, nucleophilic or electrophilic. See, the Figures (3(a)), (3(b)) and (3(c)).

In this sense, is important to note that, in this case we suspect that the more important changes in the parameters and their equalization occurs in the transition state, this can be suspect by chemical intuition, but how we can see in the different graphics this not occurs, in fact, the hardness, Fig. (1(c)), that exist a minima in $RX = -0.64230$ and a maximum in $RX = 3.21128$ this zone permit us define as a zone where the process occurs via nucleophilic attack.

In Figure (3(e)) and (3(d)) we present, the tendencies of Shannon entropy and the electron energy with the LDA approximation, E^{LDA}. In this case, the E^{LDA} increase basically in a linear way, but in the point $RX = 2.73035$ have a maximum, this maximum appears to in the chemical potential tendency. Respect to the Shannon entropy we note more structure than E^{LDA}, and in this case, we note than the Shannon entropy have a similar tendency than the electron energy, in the same form than the energy the Shannon entropy can detect the transition state, see the Figure (3(f)).

By comparison between the Shannon entropy and electron energy profiles we can note that the Shannon entropy, have a zone delimited in the region $-0.5 \leq RX \leq 0.5$, see Figure (3(f)), that have a correspondence with the transition state zone, this is an important observation, because, the Shannon entropy can detect a transition state zone, where occurs a transfer and redistribution of electron density. Comparing, the tendencies of condensed Fukui function, with the Shannon entropy tendency, we note that this zone, have a relation with a charge transfer between the methyl and the molecule and is in this zone where occurs the process of bond forming. In the same way that the condensed Fukui function, this zone is where the subtle interactions among frontier orbitals occurs, and permit to the molecular system start a complex process of the chemical bond forming, in Figure (4(a)) we present the tendency of a normal mode of vibration, and we note that, the zone predicted by the Shannon entropy exhibit a correspondence with a zone of the negative values of the frequencies, consequently, is possible that we can not speak of a specific point in the reaction path where occurs a bond breaking or bond forming. A similar argumentation, can be applied to the description of the transition state zone. Note the importance of this, is possible that, still with the modern techniques of the experimental chemistry, such the femtochemistry [19–21], we can not detect just a transition state structure, or else, a zone of transition. This zone of transition, is accoted by a zone where the Shannon entropy tendency have a slope approximately to zero, see the Figure (4(b)) accordingly, we can say that the Shannon entropy can detect and predict the zone where the most important chemical changes will be occurs, so, this kind of entropy permit us reveals some chemical aspects that are subjacent in a chemical process. Other important, observation is that the maximum of the electron energy, not correspond to the minimum of the frequencies, it is represents, probability, a conflict between the convectional interpretation, in the sense that the maximum of the energy correspond at one possible transition state structure that, in general, have the most negative value of the frequencies, but how we show in this case, this not occurs, by other hand, the minimum value of the frequencies it is related at one equality with the condensed Fukui functions, see the Figure (4(c)).

In general terms, is important to note, that the frequencies tendencies have a tree zones of negative frequencies, these Hessian values represent the transition vector which show maxima at the vicinity of the transition state. Several features are worth mentioning, the TS corresponds indeed to a saddle point, maxima at the Hessian correspond to high kinetic energy values (largest frequencies for the energy cleavage reservoirs) since they fit with maximal values in the entropy profile, and the Hessian is minimal at the TS, where the kinetic energy is the lowest (minimal molecular frequency) and it corresponds to a saddle point. In this case, the analysis of frequencies can give us, a general idea about that this mechanics occurs in tree steps, in each one, occurs some structural rearrays at expense of a decrease in

energy exchange and increased kinetic energy. It is relevant note, that the Shannon entropy, see Figure (4(b)), can detect three zones where the frequencies are negative, the first of them is between $-3.5 \leq RX \leq -2.2$ the second in $-0.5 \leq RX0.5$ and the last in $3.8 \leq RX \leq 4.0$. In the first and third zone, the Shannon entropy exhibits a change in their curvature, also, note that this last observation have a correspondence with the other parameters such, hardness, softness, chemical potential and with some Shannon entropy derivatives.

In Figure (5(b)) we compare the trend of the derivative of Snannon's entropy with respect to the number of electrons: $\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})}$ as a function of RX, with that of the DFT chemical reactivity descriptor: $\left(\frac{\partial \mu}{\partial N}\right)_{v(\mathbf{r})}$, which is associated to hardness. Even though absolute values are not the same everywhere, there is a perfect coincidence in the region close to the transition state, in terms of the RX position as well as in the absolute values.

A similar situation occurs with the derivative of Shannon's entropy with respect to the chemical potential: $\left(\frac{\partial S(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})}$, and the inverse of the Exchange energy,

$$\frac{1}{E_i^{LDA}} = -\frac{1}{\left(\frac{3}{\pi}\right)^{1/3} \int \rho(\mathbf{r})^{4/3} d\mathbf{r}},$$

see Figure (5(d)).

Finally, a plot of the derivative of Shannon's entropy with respect to the electronic energy $\left(\frac{\partial S(\mathbf{r})}{\partial E}\right)_{v(\mathbf{r})}$ as a function of RX, behaves in a manner that is remarkably similar to that of the DFT descriptor for softness: $\left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})}$ (Figure (5(f))).

The relations that were suggested above based on numerical evidence can be summarized as:

$$\left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{v(\mathbf{r})} \simeq \left(\frac{\partial \mu}{\partial N}\right)_{v(\mathbf{r})}. \tag{50}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial \mu}\right)_{v(\mathbf{r})} \simeq -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} \int \rho(\mathbf{r})^{4/3} d\mathbf{r}. \tag{51}$$

$$\left(\frac{\partial S(\mathbf{r})}{\partial E}\right)_{v(\mathbf{r})} \simeq \left(\frac{\partial N}{\partial \mu}\right)_{v(\mathbf{r})}. \tag{52}$$

From the numerical results obtained from Eqs. (50) and (52), we have been able to establish a linear relationship between the parameters involved, and the following expressions have been obtained:
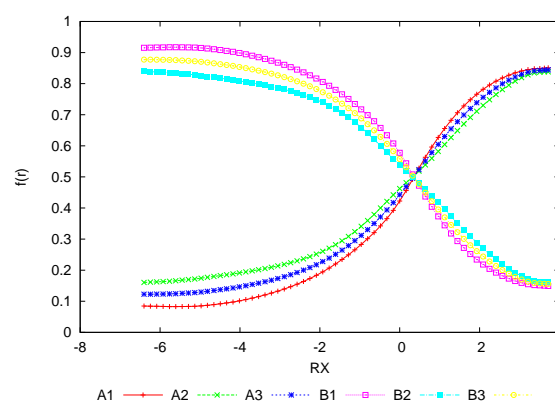
$$\text{Hardness} = \left(\frac{\partial \mu}{\partial N}\right)_{\nu(\mathbf{r})} = 28.3141 \left(\frac{\partial S(\mathbf{r})}{\partial N}\right)_{\nu(\mathbf{r})} + 0.0226, \tag{53}$$

$$\text{Softness} = \left(\frac{\partial N}{\partial \mu}\right)_{\nu(\mathbf{r})} = 24.1088 \left(\frac{\partial S(\mathbf{r})}{\partial E}\right)_{\nu(\mathbf{r})} + 0.5876, \tag{54}$$
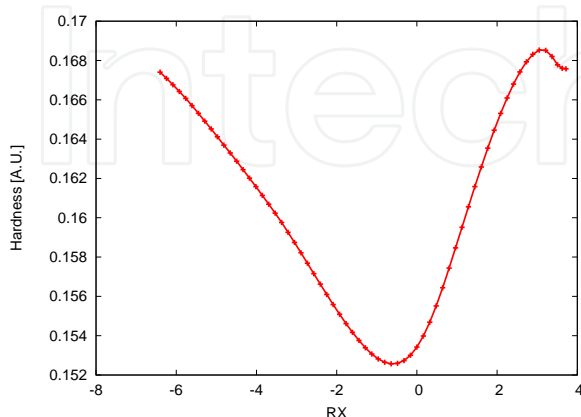
Thus, the hardness and softness values of this chemical reaction can be obtained with a good level of accuracy from the derivatives of Shannon's entropy.
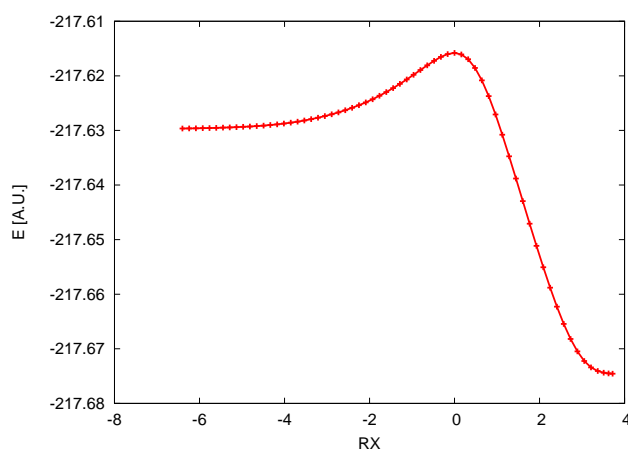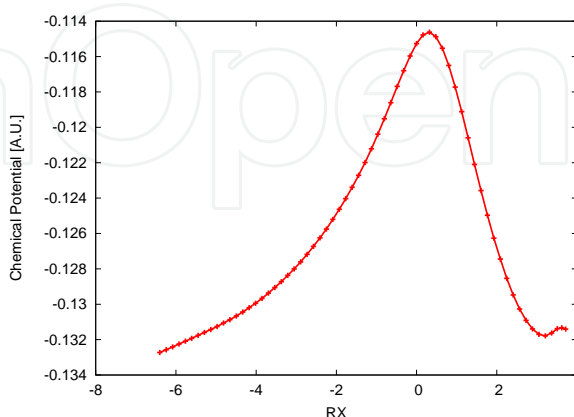

(a) Electron energy profile.

(b) Condensed Fukui function profile $A1 : f(\mathbf{r})^{-}$, $A2 : f(\mathbf{r})^{+}$, $A3 : f(\mathbf{r})$, $B1 : f(\mathbf{r})^{-}$, $B2 : f(\mathbf{r})^{+}$, $B3 : f(\mathbf{r})$, where A denote the subsystem CH_2CHF and B is the subsystem CH_3.

(c) Hardness.

(d) Chemical potential.

Figure 1. Trends of the reaction $CH_2CHF + CH_3 \rightarrow CH_3CHFCH_2$.

(a) Kinetic Energy.   (b) Exchange Energy.

(c) $RX = -0.64230$ (d) $RX = -0.32112$ (e) $RX = -0.16058$ (f) $RX = 0.00000$

(g) $RX = 0.32119$ (h) $RX = 0.48180$ (i) $RX = 0.64242$ (j) $RX = 0.96366$

(k) $RX = 1.12427$ (l) $RX = 1.44550$ (m) HOMO in
$RX = 2.08795$ (n) LUMO in
$RX = 2.08795$

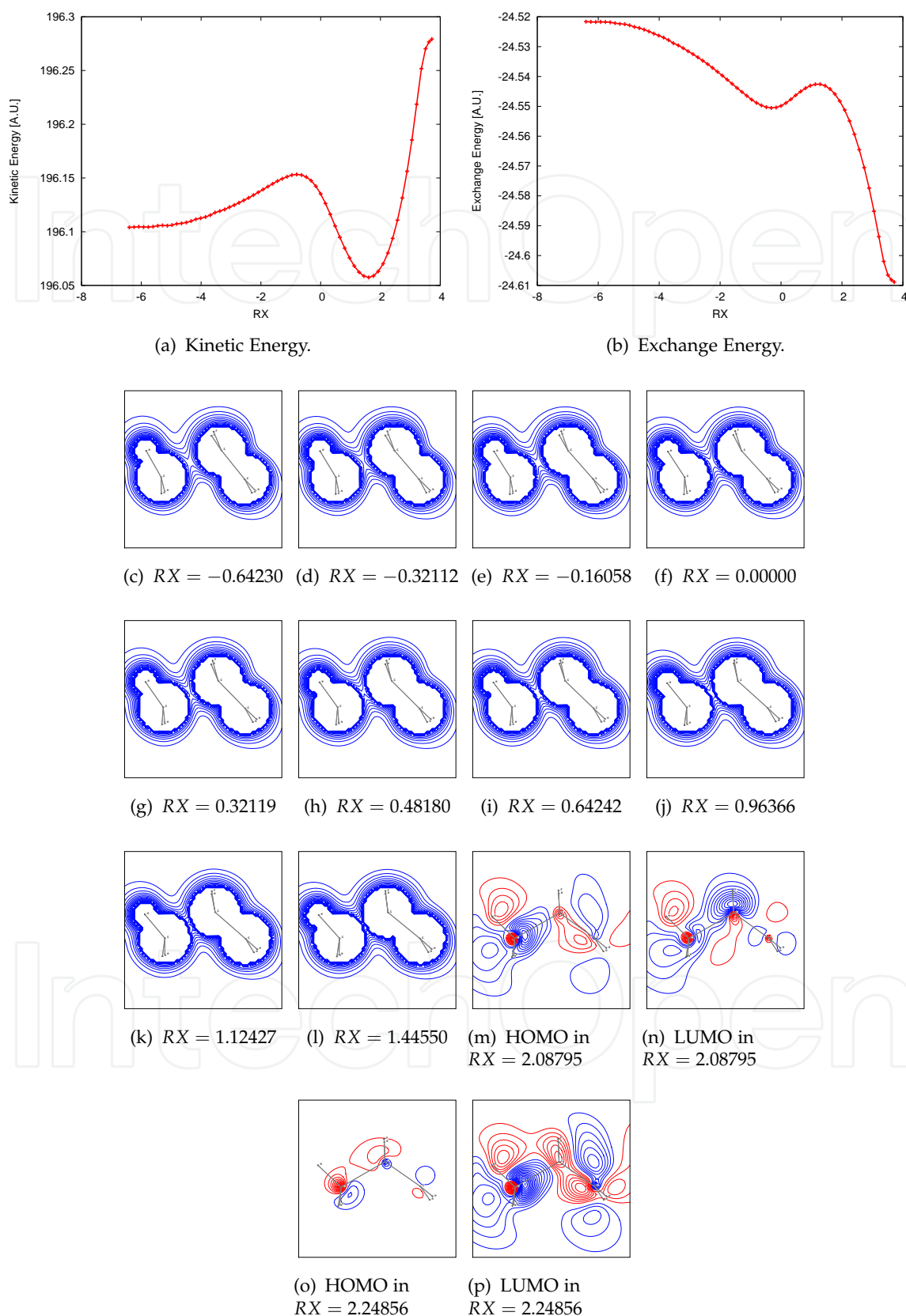(o) HOMO in
$RX = 2.24856$ (p) LUMO in
$RX = 2.24856$

Figure 2. Isosurfaces of the Molecular Electrostatic Potential, in $-0.64230 \leq RX \leq 1.44550$.

(a) HOMO, in $RX = 0.32119$

(b) LUMO, in $RX = 0.32119$

(c) MEP, in $RX = 0.32119$

(d) Exchange energy with LDA

(e) Shannon entropy
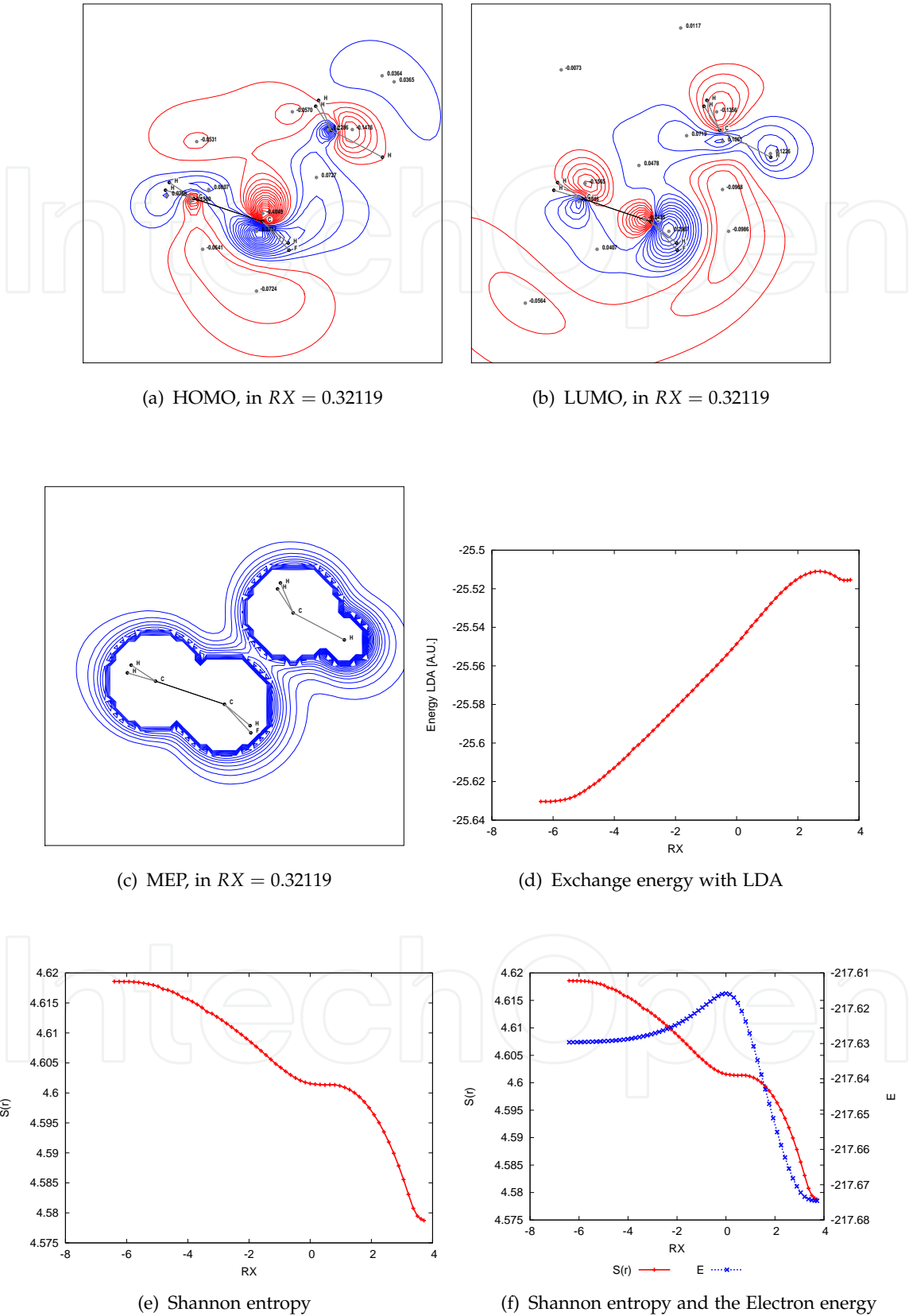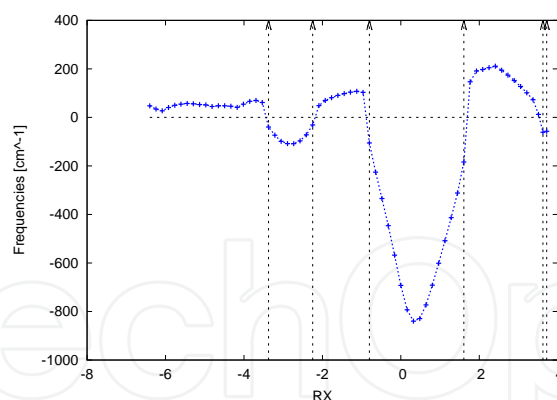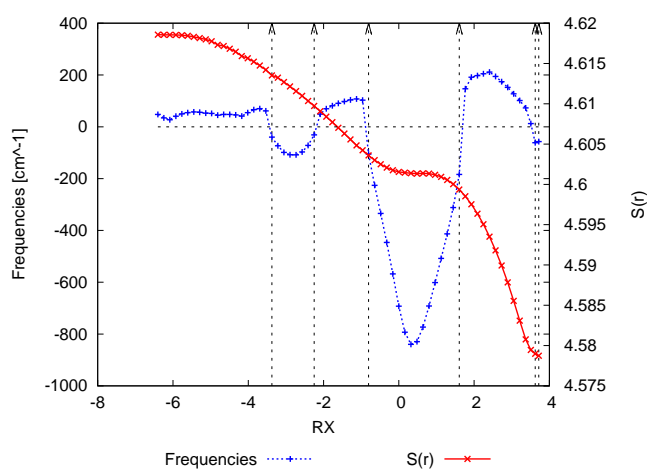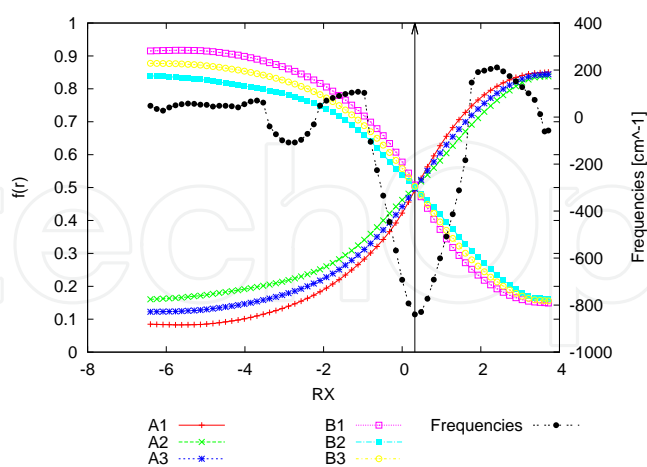

(f) Shannon entropy and the Electron energy

Figure 3. Trends of the reaction $CH_2CHF + CH_3 \rightarrow CH_3CHFCH_2$.

(a) Frequencies.

(b) Comparison between the frequencies and the Shannon entropy.

(c) Comparison between the condensed Fukui function and the Frequencies.
Where $A1 : f(\mathbf{r})^-$, $A2 : f(\mathbf{r})^+$, $A3 : f(\mathbf{r})$, $B1 : f(\mathbf{r})^-$, $B2 : f(\mathbf{r})^+$, $B3 : f(\mathbf{r})$, where A denote the subsystem CH_2CHF and B is the subsystem CH_3

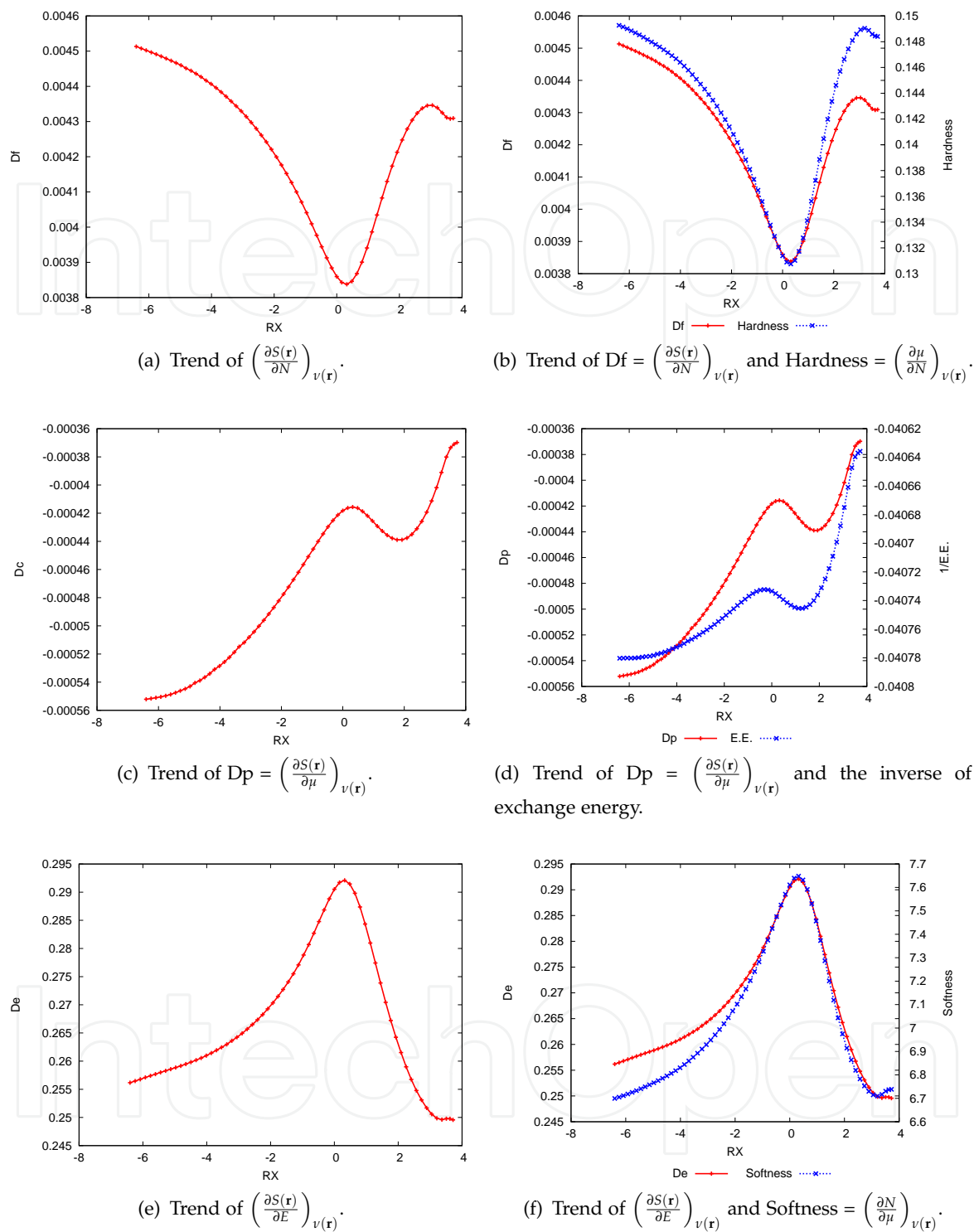**Figure 4.** Comparison among Frequencies, Shannon entropy and Fukui function.

Figure 5. Trends of the first derivatives of Shannon entropy.

3.2. Ethane conformational analysis

In this section we present a conformational analysis of ethane, as a function of the dihedral rotation angle between the two methyl groups. The initial point corresponds to the eclipsed

conformer, and an Intrinsic Reaction Coordinate analysis (IRC) has been performed, with ten degrees steps in the dihedral angle. This system was calculated in Gaussian 03 [32], using B3LYP/cc-pVTZ.

In Figure (6(a)) we present the electron energy and Shannon entropy profiles. An excellent agreement is observed between the two curves. Furthermore, a clear similarity is also observed between the behavior, along the reaction path, of the hardness and of the first derivative of Shannon's entropy with respect to the number of electrons. This is shown in Figure (6(b)).

In Figure (6(c)) we show the kinetic and exchange energies as a function of RX. Both quantities exhibit inverse behaviors,the position of the minima in one of them coinciding with the maxima of the other.

One of the most important results is shown in Figure (6(d)), where the exchange energy is plotted against Shannon's entropy along the reaction path. A perfect linear correlation is observed between these apparently unconnected quantities, leading to conclude that

i) The Shannon entropy in position space can be used as a measure of the exchange effects in molecular systems.

ii) There exists a direct relationship between the Shannon entropy and the exchange energy.

Based in these conclusions and results, a new research line is being developed, to construct a functional based on an entropic criterion.

The numerical results obtained above cab be summarized in the following manner:

$$\left(\frac{\partial S(\mathbf{r})}{\partial N} \right)_{v(\mathbf{r})} \simeq \left(\frac{\partial N}{\partial \mu} \right)_{v(\mathbf{r})}. \tag{55}$$

$$S(\mathbf{r}) \simeq -\frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} \int \rho(\mathbf{r})^{4/3} d\mathbf{r}. \tag{56}$$

The last equation suggests that there may be a fundamental connection between Chemical Density Functional Theory and Information Theory. In Table (1), we present the numerical results of Shannon's entropy and exchange energy. Using these results and a least square regression, is it possible to obtain the following linear relation between Shannon entropy and exchange energy:

$$E_e = AS(\mathbf{r}) - B, \tag{57}$$

where $A = 2.2127$ and $B = 21.0061$. With this equation, we can reproduce the Exchange Energy with a precision of 1×10^{-6}.

Angle	$S(\mathbf{r})$ [nats]	E.E. [A.U.]	$E_e = AS(\mathbf{r}) - B$ [A.U.]	precision
0	4.5902766	-10.849190	-10.8492232214	0.9999
10	4.5901580	-10.849449	-10.8494856465	0.9999
20	4.5898836	-10.850050	-10.8500928087	0.9999
30	4.5895363	-10.850815	-10.8508612761	0.9999
40	4.5892201	-10.851516	-10.8515609289	0.9999
50	4.5890276	-10.851953	-10.8519868718	0.9999
60	4.5889557	-10.852113	-10.8521459642	0.9999
70	4.5890276	-10.851953	-10.8519868718	0.9999
80	4.5892201	-10.851516	-10.8515609289	0.9999
90	4.5895363	-10.850815	-10.8508612761	0.9999
100	4.5898836	-10.850050	-10.8500928087	0.9999
110	4.5901580	-10.849449	-10.8494856465	0.9999
120	4.5902766	-10.849190	-10.8492232214	0.9999
130	4.5901580	-10.849449	-10.8494856465	0.9999
140	4.5898836	-10.850050	-10.8500928087	0.9999
150	4.5895363	-10.850815	-10.8508612761	0.9999
160	4.5892201	-10.851516	-10.8515609289	0.9999
170	4.5890276	-10.851953	-10.8519868718	0.9999
180	4.5889557	-10.852113	-10.8521459642	0.9999

Table 1. Numerical values of Shannon's entropy and Exchange Energy, in the ethane conformational analysis, where $A = 2.2127$ and $B = 21.0061$.

(a) Energy and Shannon entropy profiles

(b) Derivative of Shannon entropy and Softness profile

(c) Exchange Energy and Kinetic Energy profiles

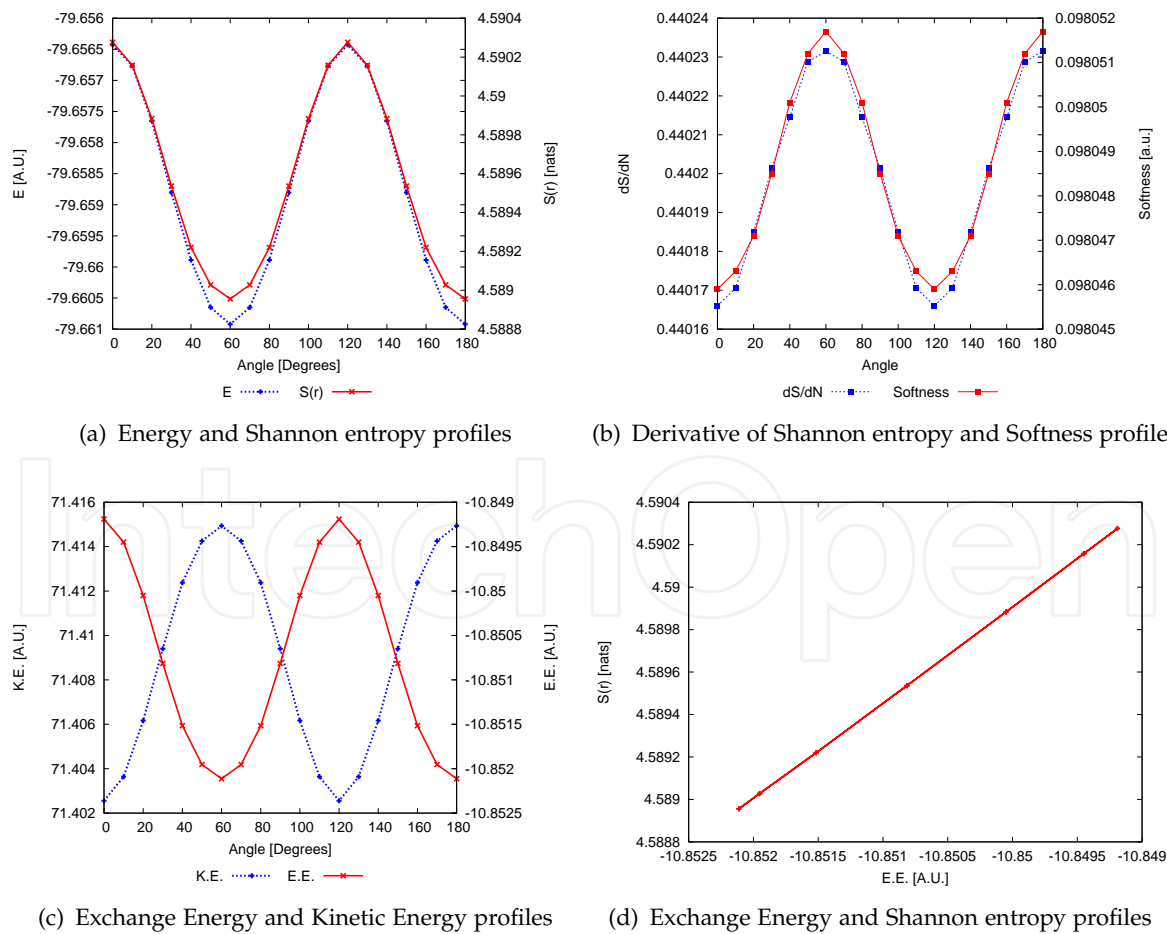(d) Exchange Energy and Shannon entropy profiles

Figure 6. Tendencies obtained for the Ethane Conformational Analysis.

4. Conclusion

In this work, I have derived relationships that connect Shannon's entropy and its derivatives, with well-known concepts in Density Functional Theory. Numerical applications of these relationships have been performed for two simple problems.

This has been permit us start a new investigation line about it, and with some this results we continue whit the study of the formalism for the construction of a functional based in a principles of physics, and the information theory, also, we pretend continue the develop of the some models that permit us find the direct relation between electron energy with the Shannon entropy.

By other hand, the application of the concepts of the information theory permit do a description more accurate than the description based in only a energetically criteria, and continue with the spirit of some works of Frieden, we speculate that is possible define or found a form that derived the DFT from some fundamental expression, that come form the Information Theory, as Frieden derivations of the fundamental equations of the Thermodynamics, or the derivation of the Scrhödinger equation.

Finally, with this example we have tried to link information from a system that is subjected to a process with the physical and chemical changes. Thus, we have linked the concept of *information*, which is an epistemological concept completely with ontological concepts and the solution concepts or interpretation of the results allows us feedback on these concepts in ontological terms, according to the author, abstract and more general.

By other part, is probable that today do not exist a ortodoxical definition of what actually is the *information*, beyond that presented by Shannon and its guidelines, criteria, characterization of it, among other things, the interpretation and the relationship with other concepts such as: energy, electron density, chemical reactivity parameters and many others need be discussed to try of establish a formal relation between concepts.

So, there is no doubt that both knowledge and the praxis and reality as knowledge scientific understanding and also, is it clear that information concept and the model itself is interdisciplinary or transdisciplinary. The concept and moreover, the model itself, promotes a systematic relation with causal analogies and parallelism with scientific knowledge, which transcends the framework of the source domain and extend in various directions, thus making the knowledge acquires an unusual resonance, as this, we believe it is feasible to complement the explanations of natural processes and natural systems.

This model is not intended that the manner of the old school, that using metaphysical substance, the particularities of the processes reveal themselves to us in the end as a progressive manifestation of homogeneous order or a unitary whole and absolute. It is simply to promote and implement a partnership scheme which promises analog route and cover knowledge in a way easier.

Acknowledgments

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