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Topological Analysis of the Fukui Function

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Abstract: In this work an alternative to the analysis of the Fukui function will be presented and compared with the traditional condensed function. The topological analysis allows us to define basins corresponding to different regions of the space, and the numerical integration of the density over those volumes gives a number amenable of a chemical interpretation in line with the Fukui function applications. Various examples are shown, a series of small molecules, a couple of clusters, and aromatic molecules. They are discussed in comparison with other methodologies and with the experimental evidence.

Introduction

In the last 25 years the development of the density functional theory of chemical reactivity has allowed introducing in a formal framework many empirical chemical concepts like electronegativity,[1] hardness,[2] Fukui function,[3] electrophilicity,[4] and others. Most of them were early defined by Parr and co-workers and are well described in ref 5. New developments were recently reviewed.[6,7] In this work, the focus will be in the Fukui function which was defined as

$$f(\vec{r}) = \left(\frac{\delta\mu}{\delta v(\vec{r})} \right)_N \tag{1}$$

where μ is the chemical potential and $v(r)$ is the external potential, and the derivative is taken at constant number of electrons N. Very early the impossibility of an exact evaluation of this derivative was realized. The energy presents a discontinuity at an integer number of electrons.[8] Therefore, one has a chemical potential from the left and another one from the right. The first corresponds to the situation where the molecule will lose charge, μ^-, and the later to the situation where the molecule will gain charge, μ^+. In the limit of zero temperature, they are exactly the

ionization potential, I, and the electronaffinity, A, respectively. Working further at that limit and using $I = E(N) - E(N-1)$ and $A = E(N+1) - E(N)$ in eq 1, we can deduce that

$$f^-(\vec{r}) = \rho_N(\vec{r}) - \rho_{N-1}(\vec{r}) \tag{2}$$

for the derivative taken from the left side, and

$$f^+(\vec{r}) = \rho_{N+1}(\vec{r}) - \rho_N(\vec{r}) \tag{3}$$

for the derivative taken from the right side. In this way, the mathematical discontinuity acquires a chemical meaning. The derivative from the left side corresponds to the capability of the molecule to donate an electron, and the derivative for the right side corresponds to the capability of accepting an electron. One further approximation has been usually done. Under the frozen orbital approximation, these equations transform into

$$f^-(r) = |\phi_H(r)|^2 \tag{4}$$

and

$$f^+(r) = |\phi_L(r)|^2 \tag{5}$$

where $\phi_H(r)$ and $\phi_L(r)$ stand for the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), respectively. The last approximation has the practical advantage of their simplicity to allow

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the calculation of the Fukui function in just one calculation to the neutral species without the necessity of calculating the charged species, especially the anions, as it is the case using eqs 2 and 3. However, their lack of relaxation effects has been lately criticized.[9,10] In the last few years, an option to calculate the Fukui function directly from eq 1 without differentiating with respect to the electron number has been put forward,[11,12] and the exact derivative with respect to the number of electrons has been also implemented.[13,14] However, as long as the currently used exchange−correlation functionals are more accurate for integer N than for fractional N,[15–17] the numerical results seem to be better for the models based in the quadratic expansion of the energy with respect to the number of electrons. Independent of the approximations used to calculate the Fukui function, all of them follow the exact equation:

$$\int f(r)\mathrm{d}r = 1 \qquad (6)$$

which is important in the use of the Fukui function as an intramolecular reactivity index. In this work, the aim is not to describe a new strategy to calculate the Fukui function but more in the way one can analyze the results of such a calculation. Very soon after the Fukui function was proposed it was realized that the analysis of a three-dimensional function is not trivial and is many times just a number for a molecule or better for a region in a molecule that is more desirable than a number for each value of $\vec{r}$. Yang and Mortier[18] coined the term "condensed" to the approximation of assigning to the Fukui function a number for each atom in the molecule. Hence, under the Mulliken population analysis approach, they proposed to approximate the Fukui function at the atom k as

$$f_k^+ = q_k(N) - q_k(N + 1) \qquad (7)$$

and

$$f_k^- = q_k(N - 1) - q_k(N) \qquad (8)$$

where $q(N + 1)$, $q(N)$ and $q(N - 1)$ are the charges at atom k on the anion, neutral, and cations species, respectively. Under the frozen orbital approximation, these expressions depend only on the electronic structure of the neutral species.[19,20] A variety of forms to calculate the charges have been presented. Most of them are based in some sort of population analysis. The arbitrariness in the way of choosing the charges has been one of the principal criticisms to the condensed Fukui function approximation.

In this work, we propose a methodologically different way to analyze the Fukui function, a topological analysis of the Fukui function, and its comparison with the most related condensation approaches.

Topological Elements to Interpret The Fukui Function. The topological analysis of the electron density was done almost three decades ago by Bader, who investigated the gradient field of the electron density to give a definition of an atom in a molecule.[21] After that, this type of analysis has been used for different functions in chemistry. Especially, Silvi and Savin[22] used it to analyze the electron localization function (ELF). The Fukui function, like the electron density and the ELF, is a scalar function in a three-dimensional (3D) space. Therefore, the analysis of its gradient field allows us to locate the critical points. The critical points of a 3D scalar function can be maximum, minimum, or saddle points. The maximum are called attractors, which are many times amenable of a physical interpretation. For instance, because of Kato's cusp condition,[23] the electron density has a maximum at the nuclei position and, therefore, the electron density has always an attractor associated to each nuclei position.[24] The cusp condition on the Fukui function was first stated by Chattaraj et al,[25] they proposed a gradient expansion for the Fukui function, lately it was derived by Ayers and Levy.[26] In the frontier molecular orbital (FMO) approximation, there is no cusp condition if the orbital has a node only at the atomic position. In this case, there is a "generalized cusp condition" for the density[27,28] depending on how many spatial nodes intersect at the atomic position. Other qualitative difference to be seen in the topological analysis is that the Fukui function calculated as the square of the frontier orbital has, of course, only the symmetries of the irreducible representation of the frontier orbital, whereas the Fukui function calculated as the density differences has all the molecule symmetries for nondegenerate states. It is also useful to define the f-localization domains, which are defined as the volume enclosed by the isosurface $f(r) = f$. It encloses all the points for which $f(r) > f$. They are reducible when they contain more than one attractor and irreducible when they contain one attractor. Each attractor is characterized by its basin, which is the set of points lying on the trajectories ending in this attractor. Since two trajectories cannot cross each other, the basins are irreducible domains, they do not overlap, and the set of all basins fills the complete space. Hence, the whole molecular space is partitioned into basins of attractors, and any physical observable can be defined into this regions. In particular, for a basin labeled, Ω_k, one can calculate the average number of electrons contained into this basin as

$$N_k = \int_{\Omega_k} \rho(\vec{r})\mathrm{d}\vec{r} \qquad (9)$$

The sum of the N_k overall basins gives, of course, the total number of electrons. Since we have a donor, f^-, and an acceptor, f^+, Fukui function, we will have two different sets of basins, $\Omega_k^\pm$, and the corresponding chemical interpretation of the resulting numbers, $N_k^\pm$, will be different, accordingly. The site with the greatest N_k^- value should be the site susceptible to donate charge, and inversely, the site with the lowest N_k^+ should be the site susceptible of accepting charge. Note that the N_k index normalizes to the number of electrons, whereas the Fukui function normalizes to one (it is an extensive quantity opposite of the condensed Fukui function). Hence, it can be used for intra- or intermolecular reactivity. However, the chemical interpretation of the N_k values needs further studies to verify its quantitative capability.
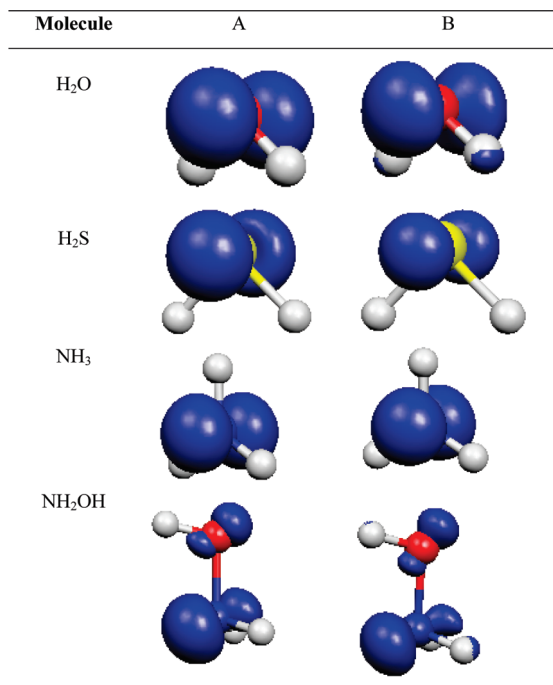
Figure 1. Isosurfaces of the donor Fukui function as (A) the square of the HOMO and (B) as the density differences.
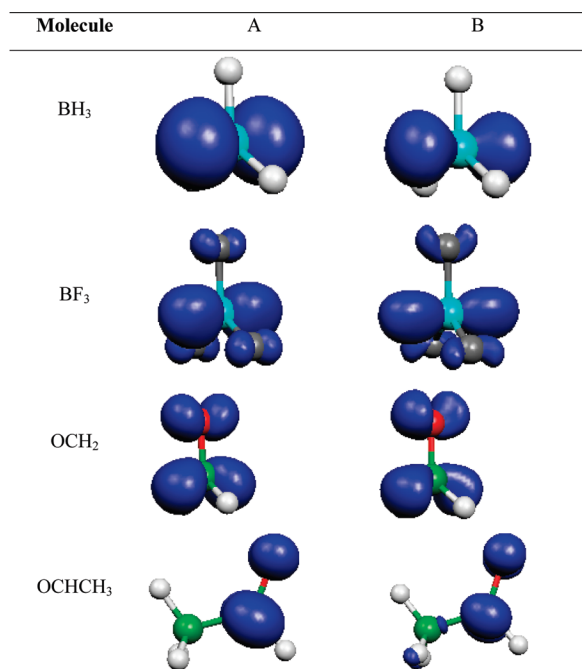
Figure 2. Isosurfaces of the acceptor Fukui function as (A) the square of the HOMO and (B) as the density differences.

One should also like to make contact with the condensed Fukui function. Hence, one can define the quantity:

$$f_k^{\pm} = \frac{N_k}{N} \qquad (10)$$

to be compared with any form of condensed Fukui function. It is to notice that eq 10 corresponds to the integration of the shape function, $\sigma(\vec{r}) = \rho(\vec{r})/N$, over the basins of the Fukui function.[29] To avoid the basis set dependence of most

Table 1. Average Number of Electrons on the Basins of the Donor Fukui Function Calculated as the Square of the HOMO, A, and as the Density Differences, B, at B3LYP/6-311g** and B3LYP/6-311++g**

| molecule | atomic basin | A | | B | |
		BS1[a]	BS2[b]	BS1[a]	BS2[b]
H₂O	O	10.0	10.0	8.46	8.46
H₂S	S	18.0	18.0	16.0	16.0
HCN	C	6.6	6.6	5.6	5.6
	N	7.4	7.4	7.2	7.2
CO	C	5.7	5.7	5.2	5.2
NH₂⁻	N	10.0	10.0	8.4	8.4
NH₃	N	10.0	10.0	7.8	7.8
NH₂OH	N	8.69	8.72	6.86	6.90
	O	7.93	7.94	7.66	7.61
NH₂F	N	9.08	9.09	7.19	7.25
NHF₂	N	8.45	8.45	6.86	6.96
NF₃	N	8.02	8.02	6.56	6.66

[a] BS1 is B3LYP/6-311g**. [b] BS2 is B3LYP/6-311++g**.

Table 2. Average Number of Electrons on the Basins of the Acceptor Fukui Function Calculated As the Square of the LUMO, A, and as the Density Differences, B, at B3LYP/6-311g** and B3LYP/6-311++g**

| molecule | atomic basin | A | | B | |
		BS1[a]	BS2[b]	BS1[a]	BS2[b]
BH₃	B	8.0	8.0	5.8	5.7
BH₂F	B	7.37	7.34	5.45	5.56
BHF₂	B	6.84	6.79	5.24	5.78
BF₃	B	6.51	9.8	7.7	7.1
BCl₃	B	8.10	8.16	5.67	5.88
CH₃⁺	C	8.03	8.03	5.29	5.64
CF₃⁺	C	6.94	6.90	5.21	5.37
CCl₃⁺	C	7.89	7.89	5.96	5.93
CBr₃⁺	C	7.85	7.85	5.93	5.93
CI₃⁺	C	6.28	6.26	5.75	5.75
CO	C	6.28	6.26	5.93	5.92
OCH₂	C	7.87	7.83	6.08	5.92
OCHCH₃	C1	8.94	8.68	6.45	6.51

[a] BS1 is B3LYP/6-311g**. [b] BS2 is B3LYP/6-311++g**.

population analysis, we condense the Fukui function integrating over its own basins:[30]

$$f_{k,C}^{\pm} = \int_{\Omega_k} f_k^{\pm}(\vec{r}) d\vec{r} \qquad (11)$$

Assuming one has the topology of the basins to give them a chemical interpretation, the average number of electrons on them, to quantify the capability of a site to accept or donate charge and is analogous to a condensed Fukui function to compare with.

Results and Discussion

The molecular geometries have been optimized using the B3LYP density functional method[31] and two different basis sets,[32,33] namely 6-311G** and 6-311++G**, denoted in the tables as BS1 and BS2, respectively. The two different basis sets have been used to prove that the results are not sensitive to the use of diffuse function. All electronic structure calculations were done using the Gaussian 03 program,[34] the topological analysis of the scalar functions,

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Table 3. Condensed Donor Fukui Function, using eqs 10 and 11, for the Two Methodologies[a]

molecule	atom	A		B	
		eq 10	eq 11	eq 10	eq 11
H_2O	O	1.00	1.00	0.84	0.78
H_2S	S	1.00	1.0	0.9	0.9
HCN	C	0.47	0.44	0.40	0.43
	N	0.53	0.56	0.51	0.46
CO	C	0.41	0.86	0.37	0.67
NH_2^-	N	1.0	1.0	0.84	0.82
NH_3	N	1.00	1.00	0.78	0.77
NH_2OH	N	0.48	0.76	0.38	0.47
	O	0.44	0.19	0.42	0.21
NH_2F	N	0.51	0.80	0.40	0.59
NHF_2	N	0.325	0.54	0.26	0.50
NF_3	N	0.23	0.64	0.19	0.41

[a] The square of the HOMO, A, and the density difference, B, at the B3LYP/6-311++g** level of calculation.

Table 4. Condensed Acceptor Fukui Function, using eqs 10 and 11, for the Two Methodologies[a]

molecule	atom	A		B	
		eq 10	eq 11	eq 10	eq 11
BH_3	B	1.00	1.00	0.72	0.8
BH_2F	B	0.46	0.89	0.34	0.86
BHF_2	B	0.28	0.82	0.22	0.88
BF_3	B	0.3	0.9	0.24	0.9
BCl_3	B	0.14	0.64	0.10	0.35
CH_3^+	C	1.00	1.00	0.70	0.71
CF_3^+	C	0.21	0.62	0.17	0.40
CCl_3^+	C	0.14	0.50	0.11	0.22
CBr_3^+	C	0.071	0.49	0.054	0.19
CI_3^+	C	0.24	0.50	0.22	0.15
CO	C	0.45	0.75	0.42	0.83
OCH_2	C	0.49	0.67	0.37	0.68
$OCHCH_3$	C1	0.36	0.50	0.27	0.39

[a] The square of the HOMO, A, and density difference, B, at the B3LYP/6-311++g** level of calculation.

and the calculations of the condensed Fukui function were done with the DGrid 4.4 set of programs.[35]

Figures 1 and 2 show for some molecules the representative isosurfaces of the donor and acceptor Fukui function, respectively. One can see that qualitatively in all cases the functions are very similar, presenting high similarity with the frontier orbital shapes. It is to note that this result is valid only when one analyzes the chemically meaningful Fukui function, i.e., the f^+ and f^- for the acceptor and the donor molecules, respectively. However, there are many cases where the differences can be significant.[36,37] Therefore, for a more exhaustive evaluation, it is important to have a methodology to quantify the Fukui function at the reactive sites of a molecule. This is the main point of this work, to introduce the topological analysis of the Fukui function.

In Table 1, one can see the average electron population of each basin of the donor Fukui function, eq 9, for a series of donor molecules calculated with the different methodologies and with two different basis sets. One notes that, contrary to the calculations based on population analysis, the results are almost independent of the basis set. In general, the numbers calculated integrating over the basins associated to the square of the HOMO, A in Figures 1 and 2, are greater than the ones calculated integrating over the basins associated to the density differences, B in Figures 1 and 2. In particular, using the square of the HOMO, the hydrogen atoms give all the charge to the basin associated to the heteroatom. Hence, for molecules, like H_2O and NH_3, the basin associated to the heteroatom has the total electron numbers of the molecule. However, the qualitative trends are the same. For example, comparing a series of molecules, like NH_2F, NHF_2, and NF_3, the tendency is the same. Only one exception exists in this series of molecules. For the NH_2OH molecule, the Fukui function calculated as the square of the HOMO predicts the nitrogen atom as the most reactive, whereas the Fukui function calculated as the density differences predicts

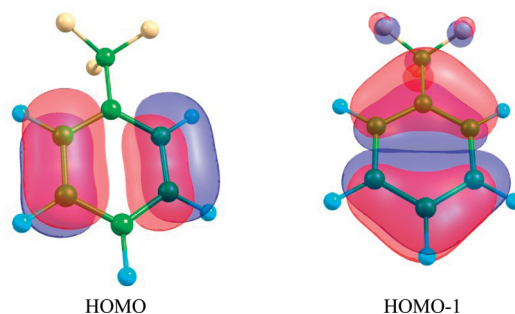**Table 5.** Condensed Donor Fukui function, using eqs 9 and 11, for the Two Methodologies[a]

compound C_6H_5X	position (k)	A		B		f_k^- [b]	observed products, % per site[c]		
		eq 9	eq 11	eq 9	eq 11		nit.	benz.	brom.
	o	6.65	0.08	4.93	0.06	0.12	28.5	43.5	19.9
CH_3	m	6.20	0.05	4.69	0.04	0.05	1.5	4.5	0
	p	8.40	0.34	6.75	0.20	0.03	40	52	60.3
	o	7.54	0.12	5.84	0.51	0.13			
NH_2	m	5.20	0.001	5.12	0.02	0.03			
	p	9.48	0.28	4.98	0.20	0.23			
	o	7.32	0.12	5.64	0.09	0.12	20		4.9
OH	m	5.34	0.02	5,2	0.03	0.06	0		0
	p	8.92	0.32	6.9	0.22	0.27	6090.2		
	o	7.66	0.14	6.0	0.10	0.14			
OCH3	m	4.26	0.01	4.9	0.01	0.02			
	p	9.60	0.3	7.02	0.19	0.25			
	o	8.40	0.26	4.61	0.04	0.16			
CF_3	m	7.00	0.24	4.90	0.05	0.17			
	p	0.00	0.00	6.70	0.20	0.16			
	o	6.53	0.06	4.86	0.05	0.16			
C≡N	m	6.2	0.05	4.77	0.04	0.15			
	p	8.24	0.29	6.62	0.19	0.13			
	o	10.3	0.25	5.98	0.14	0.15	0.3		0
NO_2	m	10.38	0.24	6.34	0.15	0.17	93.2		100
	p	0.00	0.00	3.06	0.00	0.16	6.40		

[a] The square of the HOMO, A, and density difference, B, at the B3LYP/6-311++g** level of calculation. [b] See ref 39 and 40. [c] See ref 41.

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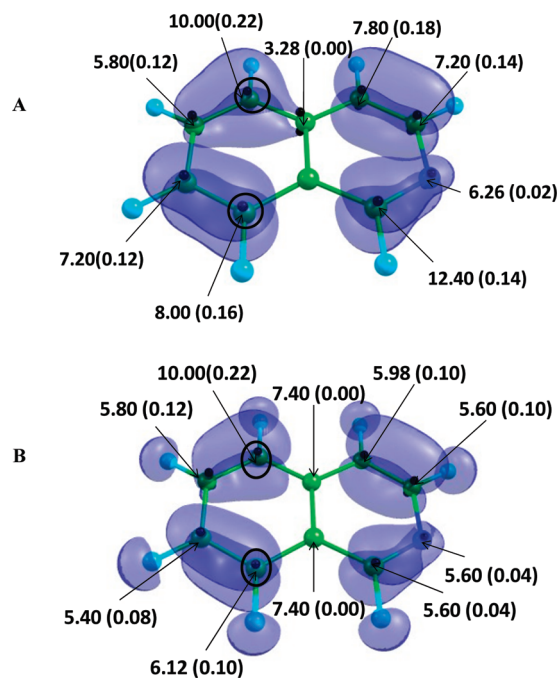
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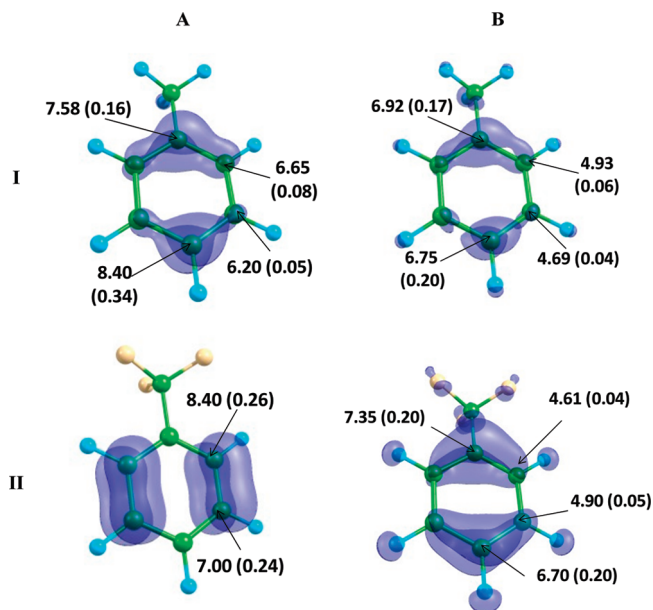
Figure 3. Isosurfaces of the donor Fukui function (A) as the square of the HOMO and (B) as the density differences. Condensed Fukui functions using eqs 9 and 11 in parentheses for (I) $C_6H_5CH_3$ and (II) $C_6H_5CF_3$ molecules at the B3LYP/6-311++G** level of calculation.

Figure 4. Isosurfaces of the HOMO and HOMO-1 for $C_6H_5CF_3$ at the B3LYP/6-311++G** level of calculation.

Figure 5. Isosurfaces of the donor Fukui function as (A) the square of the HOMO and (B) as the density differences. Condensed Fukui functions using eqs 9 and 11 in parentheses, enclosed by circles are the experimentally more reactive carbons.

the oxygen atom as the most reactive. Experimentally, there is evidence that the nitrogen atom is the most reactive, at least, for protonation, an addition of a carbocation.[38] In Table 2, a similar analysis is shown for the acceptor Fukui function in a series of Lewis acids. Again, the results are very independent of the basis set, and the values calculated using the square of the LUMO are always greater than the values calculated using the density differences. There is one exception for the BF_3 molecule, the values show a great dependence on the basis set, especially the ones calculated using the square of the LUMO. The reason is simple. Changing the basis set changes the order of the virtual orbitals, and the LUMO's are not the same. Hence, the effect is more pronounced in the Fukui function calculated with the LUMO. However, also in this case, looking at any family of molecules the trends are similar. It is important to observe that the interpretation of the numbers is now different. It seems that the most reactive molecule or site is not the one with the biggest number, as it is the case with the condensed Fukui function. Now, the most reactive molecule or site seems to be the one with the smallest number, as it can be seen in the series BH_3, BH_2F, and BHF_2. The apparent failure of this rule in the BHF_2 molecule using the 6-311++G** basis set is due to the numerical difficulty to find a basin associated to the hydrogen atom. Hence, all the charge is added to the basin associated to the boron atom. The BF_3 molecule is ruled out because of the explained change in the frontier orbital. It is important to mention that, independent of the procedure used to calculate the Fukui function, the acceptor Fukui function will be always more difficult to calculate accurately. This is due to the dependence on the virtual frontier orbital and to the complications of correctly calculating the density of an anion. The empirical rule presented here needs further study.

To make contact with the commonly used condensed Fukui function, we have calculated a related quantity given by eq 10 to compare with. The results are in Tables 3 and 4 for the donor and acceptor Fukui functions, respectively. Regarding the donor Fukui function, one can see that the numbers are different, but the trends are similar with the exceptions of CO and NH_2OH molecules where even the trends are different. Remember, however, that the prediction of the correct polarization in the CO molecule is difficult for any methodology. The comparison of the acceptor Fukui function is more difficult because the interpretation of the numbers is different. The condensed Fukui function of eq 11 predicts the most reactive site as the one with the greatest value. Whereas the number associated to eq 10 is the opposite one, with the smallest value for the most reactive site.

In Table 5, the models presented in this work are compared with the condensed Fukui function according to eqs 9 and 11. A set of monosubstituted benzenes have been chosen, C_6H_5X, X = CH_3, NH_2, OH, and OCH_3 (electron-releasing
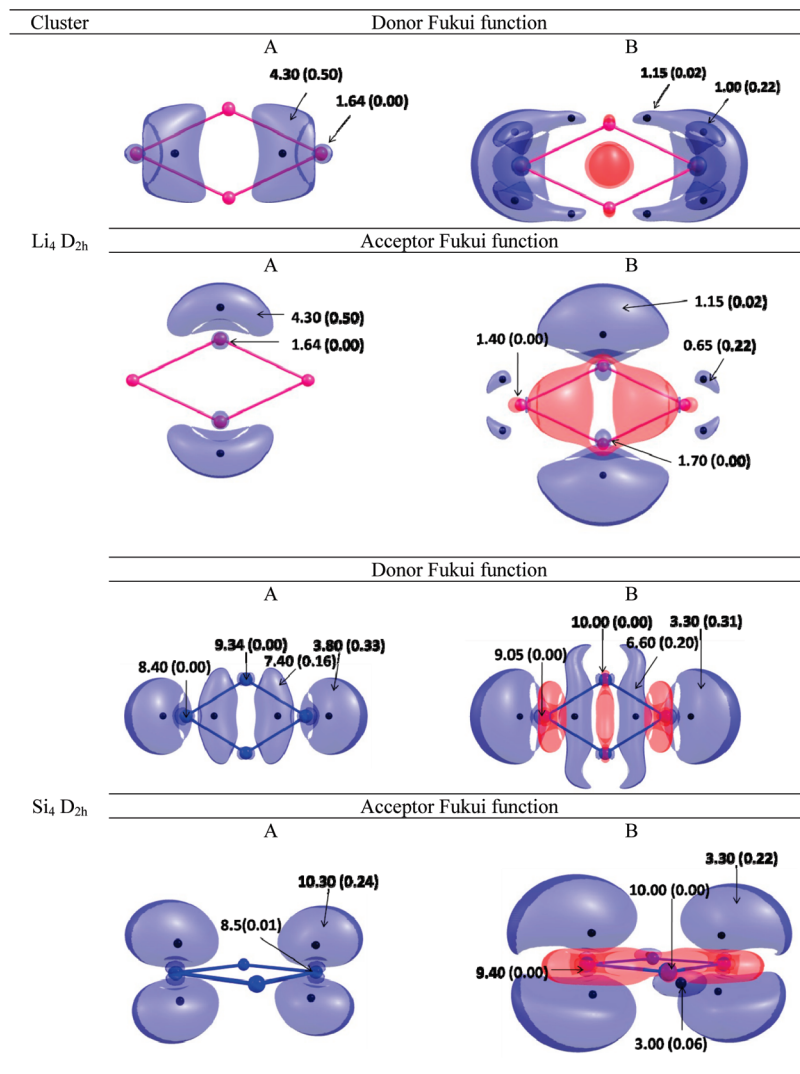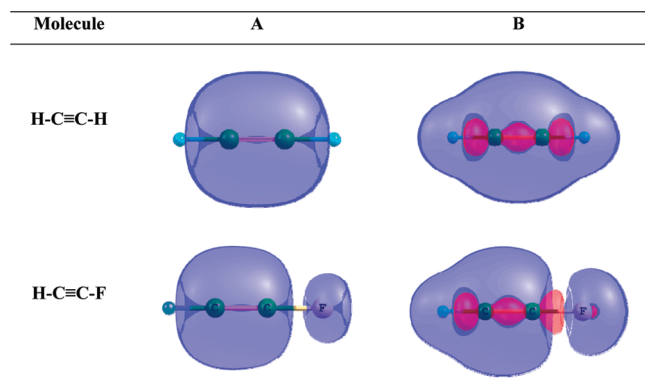
Figure 6. Isosurfaces of the donor Fukui function (A) as the square of the HOMO and (B) as the density differences. Condensed Fukui functions using eqs 9 and 11 in parentheses for Li_4 and Si_4 clusters at the B3LYP/6-311++G** level of calculation.

substituent) and X = CF_3, CN, and NO_2 (electron-attracting substituent). In general, all values show the same qualitative trends, which have also been studied before.[39–41] Note, that in the cases the HOMO is degenerated, it is necessary to consider an average among them.

The isosurfaces and condensed values of the Fukui functions (A and B approximations) to the $C_6H_5CH_3$ (*ortho−para* reactivity) and $C_6H_5CF_3$ (*meta* reactivity) are shown in parts I and II of the Figure 3; the condensed values were obtained using eqs 9 and 11. Excluding the *ipso* position in the $C_6H_5CH_3$ reactivity rank, carbons in position *ortho* and *para* are the next more reactive positions, with the *para* position as the most reactive between them, which is in agreement with the experimental observations. When we analyze the results to the $C_6H_5CF_3$ (*meta* reactivity), there are clearly differences between both methods. To evaluate whether this difference is due to an inadequate energy ordering of the orbitals or not, we have explored the lowest energy orbitals. Figure 4 shows the isosurfaces of the HOMO and HOMO-1 orbitals, and comparing with the Figure 3, we can see that the topology of the HOMO-1 orbital is similar to the Fukui function isosurface obtained by the finite

differences approximation (method B). Hence, it is important to remark that to obtain an adequate description of reactivity in agreement with the experimental observations, it is necessary the use the HOMO and HOMO-1 orbitals in the Fukui function calculation at the frozen orbital approximation, even when they are not strictly degenerates. The use of the HOMO-1 orbital has been earlier empirically used[41] and recently formally justified.[42]

Sometime ago, Dewar discussed some examples of molecules where the FMO approximation fails to adequately describe regioselectivity.[43] Those molecules were recently studied by Ayers et al[37] using density functional chemical reactivity concepts like the ones analyzed in this work. Therefore, one of these molecules, isoquinoline, has been taken as an example, and the results are shown in Figure 5. The most reactive carbon atoms are enclosed by a circle. Leaving aside the ipso reactions, which are energetically unfavorable, one can see that the finite difference approximation gives results in qualitative agreement with the experimentally observed reactivity. The model based in the square of the HOMO fails as it was predicted and explained by Dewar[43] and lately by Ayers.[37] Qualitatively, one can try to

| Molecule	A	B
H–C≡C–H		
H–C≡C–F		

Figure 7. Isosurfaces of the donor Fukui function (A) as the square of the HOMO and (B) as the density differences.

understand the difference because the models based on the finite difference approximation take into account the covalent effect, through the topology of the Fukui function, and the electrostatic effects through the integration of the total density over the basins.

Other important chemical species which have been extensively studied in the last few years are the atomic clusters.[44] The local reactivity of some clusters has been theoretically addressed using different methodologies to calculate the Fukui functions.[30,45–49] Figure 6 shows the

Fukui function isosurfaces for the Li_4 and Si_4 clusters obtained by A and B approximations and the corresponding condensed values calculated by eqs 9 and 11. One can see that the principal difference between A and B approximations are the number of basins, but in general, the qualitative reactivity information is the same.

Another important point to study through a topological analysis is the existence of regions with a negative value of the Fukui function.[9,50] Of course, under the approximation of frozen orbitals, this is not possible. However, going beyond this approximation, there is in fact regions of negative values.[10] Figure 7 shows some isosurfaces of the Fukui function for the acetylene molecule and one nonsymmetric derivative. The color now indicates the sign of the Fukui function. Blue means positive, and red means negative. Model A which is the frozen orbital approximation shows, as expected, only positive values. However, in all molecules, the Fukui function in model B, with relaxation effects, presents a region of negative values. There is always a plane containing the atoms into the region of the triple bond which has a negative value of the Fukui function. It seems that in the core region is always probable to find negative values because of the orthogonalization restrictions. A more difficult question is the existence of a basin completely contained in the negative region. Unfortunately, the numerical accuracy
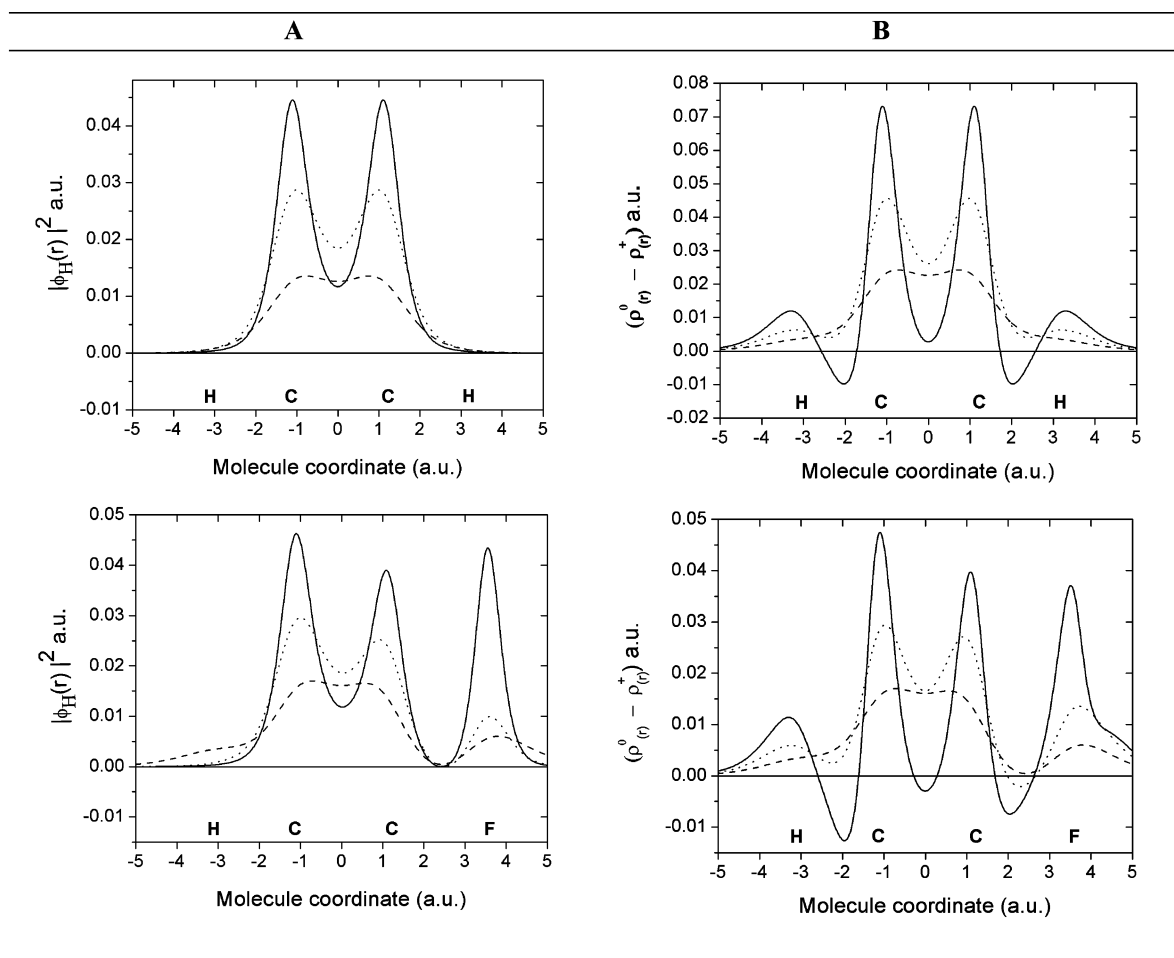
Figure 8. Values of the Fukui function, in atomic units, calculated (A) as the square of the HOMO and (B) as the density differences. Continuous, dot, and dash curves stand for calculated values at distance of 0.5, 1.0, and 1.50 au from the molecular axes.

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Table 6. Average Number of Electrons on the Basins of the Donor Fukui Function Calculated as the Square of the HOMO, A, and as the Density Differences, B, at B3LYP/6-311g** and B3LYP/6-311++g**

		A		B	
molecule	atom	BS1[a]	BS2[b]	BS1[a]	BS2[b]
H−C≡C−H	C_1	7.00	7.00	5.83	5.83
	C_2	7.00	7.00	5.83	5.83
H−C≡C−F	C_1	7.18	7.16	6.09	6.05
	C_2	5.96	5.97	5.50	5.55

[a] BS1 is B3LYP/6-311g**. [b] BS2 is B3LYP/6-311++g**.

to answer the question is too high. Figure 8 shows the values of the Fukui function calculated at distance of 0.5, 1.0, and 1.50 au from the molecular axes. One can see that, beyond the frozen orbital approximation, model B, the Fukui function shows various minima at distance of 0.5 au which, however, disappears rapidly when the function is evaluated at greater distances with respect to the molecular axes. More specific, there are critical points of different ranges and not precisely an attractor. It is also interesting to note that the attempts to reduce the function to a collection of numbers lost information. Table 6 has the values of the integration of the density over the basins. One can see that the integrated numbers cannot distinguish between both models, A and B. Even though Figure 8 shows clearly that both functions are different.

Resuming, the topological analysis of the Fukui function seems to be an alternative to the condensed version of the Fukui function, and it has the advantage of being mathematically clearly defined, avoiding the ambiguities in the form of condensing the Fukui function.

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