Electron Localization Function at the Correlated Level: A Natural Orbital Formulation [*Journal of Chemical Theory and Computation* **2010**, *6*, 2736–2742 DOI: 10.1021/ct1003548].

Ferran Feixas, Eduard Matito,* Miquel Duran, Miquel Solà, and Bernard Silvi*

In a paper recently published,[1] we stated that Piris had developed a functional which did not fulfill either the sum rules or the antisymmetry requirements. The formula we gave was wrong. The actual formula we should have written is

$$\pi(\mathbf{r}_1, \mathbf{r}_2) = \sum_i \sum_{j,i} n_i n_j \, \varphi_i^*(\mathbf{r}) \, \varphi_j^*(\mathbf{r}_2) \, \varphi_i(\mathbf{r}_1) \, \varphi_j(\mathbf{r}_2)$$
$$- \sum_i \sum_{j \neq i} \sqrt{n_i n_j} \, \varphi_i^*(\mathbf{r}_1) \, \varphi_j^*(\mathbf{r}_2) \, \varphi_j(\mathbf{r}_1) \, \varphi_i(\mathbf{r}_2)$$
$$- \sum_i^{nco} \sum_{j \neq i}^{nco} \sqrt{(1-n_i)(1-n_j)} \, \varphi_i^*(\mathbf{r}_1) \, \varphi_j^*(\mathbf{r}_2) \, \varphi_j(\mathbf{r}_1) \, \varphi_i(\mathbf{r}_2)$$
$$+ 2 \sum_{i,j > nco} \sum_{j \neq i} \sqrt{n_i n_j} \, \varphi_i^*(\mathbf{r}_1) \, \varphi_j^*(\mathbf{r}_2) \, \varphi_j(\mathbf{r}_1) \, \varphi_i(\mathbf{r}_2)$$
$$- \frac{1}{2} \sum_i n_i^2 \varphi_i^*(\mathbf{r}_1) \, \varphi_i^*(\mathbf{r}_2) \, \varphi_i(\mathbf{r}_1) \, \varphi_i(\mathbf{r}_2)$$

where nco is the number of occupied HF orbitals, and which does not fulfill the sum rule. Notice this is not the expression of PNOF1,[2] which attains both the sum rule and the antisymmetry prescriptions, but a particular application of PNOF1 that one can deduce from eqs 61, 62, and 40 in ref 2. PNOF1 depends upon a matrix (Δ) which is not specified and thus cannot be used, except for the particular application we just mentioned. However, this one is not convenient for the calculation of the electron localization function (ELF) because it fulfills neither the sum rule nor provides a correct description of the Fermi hole. The recently developed PNOF2,[3] PNOF3,[4] and PNOF5[5] functionals also fulfill the aforementioned requirements, and in principle, they could be used for the computation of the pair density needed in the calculation of the ELF.

This functional was not used for the calculations presented in the paper, and thus the conclusions drawn in the paper hold. We apologize for this mistake and thank Prof. Mario Piris for noticing this error.

■ REFERENCES

(1) Feixas, F.; Matito, E.; Duran, M.; Solà, M.; Silvi, B. *J. Chem. Theory Comput* **2010**, *6*, 2736–2742.

(2) Piris, M. *Int. J. Quantum Chem.* **2006**, *106*, 1093–1104.

(3) Piris, M.; Lopez, X.; Ugalde, J. *J. Chem. Phys.* **2007**, *126*, 214103.

(4) Piris, M.; Matxain, J.; Lopez, X.; Ugalde, J. *J. Chem. Phys.* **2010**, *132*, 031103.

(5) Piris, M.; Matxain, J.; Lopez, X.; Ugalde, J. *J. Chem. Phys.* **2010**, *133*, 111101.

ACS Publications

1231

dx.doi.org/10.1021/ct2001123 | *J. Chem. Theory Comput.* 2011, 7, 1231–1231