



Correction: Why local softness and local hyper-softness are more appropriate local reactivity descriptors than dual descriptor and Fukui functions?

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Correction to:

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After Eq. (23), the sequence of inequalities has an extra 1/2 factor:
According to working Eqs. (2) and (3), the inequality (23) is:

$$\begin{aligned} \frac{1}{2}\gamma \cdot \eta^{-3} &< \eta^{-2} \\ \frac{1}{2}\gamma \cdot S^3 &< S^2 \\ \frac{1}{2}\gamma \cdot S^3 &< S^2 \quad / \cdot |f^{(2)}(\mathbf{r})| \\ |f^{(2)}(\mathbf{r})| \cdot \frac{1}{2}\gamma \cdot S^3 &< |f^{(2)}(\mathbf{r})| \cdot S^2 \end{aligned} \quad (24)$$

Again, we know that the working formula to get the Fukui function $f(\mathbf{r})$ can be given by any of the three working equations that define the Fukui function as indicated by Eq. (6). Since:

$$\begin{aligned} |f^{(2)}(\mathbf{r})| &< 1, \\ 0 &< f^+(\mathbf{r}) < 1, \\ 0 &< f^-(\mathbf{r}) < 1, \text{ and} \\ 0 &< \bar{f}(\mathbf{r}) < 1, \end{aligned}$$

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we can replace $|f^{(2)}(\mathbf{r})| < 1$ with $f^+(\mathbf{r})$, $f^-(\mathbf{r})$, or $\bar{f}(\mathbf{r})$ in the inequality (24):

$$f(\mathbf{r}) \cdot \frac{1}{2}\gamma \cdot S^3 < |f^{(2)}(\mathbf{r})| \cdot S^2 \quad (25)$$

That is not correct because the 1/2 factor is already included in the definition of γ as indicated in the Eq. (3):

$$\gamma[N, v(\mathbf{r})] \equiv \left(\frac{\partial^3 E}{\partial N^3} \right)_{v(\mathbf{r})} = \frac{1}{2} (I_1 + A_1 - I_2 - A_2)$$

As a consequence, $\gamma = \frac{1}{2} (I_1 + A_1 - I_2 - A_2)$ is correct and not $\frac{1}{2}\gamma = \frac{1}{2} (I_1 + A_1 - I_2 - A_2)$

The correct writing is as follows:

According to working Eqs. (2) and (3), the inequality (23) is:

$$\begin{aligned} \gamma \cdot \eta^{-3} &< \eta^{-2} \\ \gamma \cdot S^3 &< S^2 \\ \gamma \cdot S^3 &< S^2 \quad / \cdot |f^{(2)}(\mathbf{r})| \\ |f^{(2)}(\mathbf{r})| \cdot \gamma \cdot S^3 &< |f^{(2)}(\mathbf{r})| \cdot S^2 \end{aligned} \quad (24)$$

Again, we know that the working formula to get the Fukui function $f(\mathbf{r})$ can be given by any of the three working equations that define the Fukui function as indicated by Eq.(6). Since:

$$\begin{aligned} |f^{(2)}(\mathbf{r})| &< 1, \\ 0 &< f^+(\mathbf{r}) < 1, \\ 0 &< \bar{f}(\mathbf{r}) < 1, \text{ and} \\ 0 &< f^-(\mathbf{r}) < 1, \end{aligned}$$

we can replace $|f^{(2)}(\mathbf{r})| < 1$ with $f^+(\mathbf{r})$, $f^-(\mathbf{r})$, textitor $\bar{f}(\mathbf{r})$ in the inequality (24):

$$f(\mathbf{r}) \cdot \gamma \cdot S^3 < |f^{(2)}(\mathbf{r})| \cdot S^2 \quad (25)$$

This correction does not invalidate the demonstration that leads to Eq. (24) because the Eq. (23) is the end of the demonstration and the next lines correspond to simple replacements of the $\frac{1}{2} (I_1 + A_1 - I_2 - A_2)$, $(I_1 - A_1)^{-3}$, and $(I_1 - A_1)^{-2}$ with γ , η^{-3} , and η^{-2} , respectively. Finally, since $\eta^{-1} = S$, the replacement finishes when, η^{-3} , and η^{-2} are expressed as S^3 , and S^2 , respectively.

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