THE JOURNAL OF PHYSICAL CHEMISTRY C
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCC

Addition/Correction

Correction to "Going Beyond the Limits of Classical Atomistic Modeling of Plasmonic Nanostructures"

Piero Lafiosca, Tommaso Giovannini, Michele Benzi, and Chiara Cappelli*

J. Phys. Chem. C **2021**, *125* (43), 23848−23863. DOI: 10.1021/acs.jpcc.1c04716

Cite This: https://doi.org/10.1021/acs.jpcc.3c01565

Read Online

ACCESS | Metrics & More | Article Recommendations

In the original paper, the Fermi energy values ε_F are incorrect. This affects the data in Figure 5 and the discussion of numerical results. As reported in ref 29, the Fermi energy can be computed from n_{2D}, i.e., graphene 2D electron density (see eq 8 in the original paper) by exploiting the following equation:

$$\varepsilon_F = \hbar v_F \sqrt{\pi n_{2D}} \tag{1}$$

where $\hbar$ is the reduced Planck constant and v_F is the Fermi velocity. The 3D atomic effective electron density n_0 can be computed as

$$n_0 = \frac{\tilde{n}_0}{m^*} \tag{2}$$

where $\tilde{n}_0$ is the 3D atomic electron density and m^* is the effective electron mass, which in the case of metallic nanostructures is usually approximated to 1. However, for graphene-based materials, n_0 can be obtained from the 2D electron density by assuming that (see ref 29 in the original paper):

$$\tilde{n}_0 = n_{2D} \cdot a_0,\ m^* = \frac{\sqrt{\pi n_{2D}}}{v_F}$$

where a_0 is the Bohr radius. By replacing such definitions in eq 2 we obtain

$$n_0^{\text{graphene}} = \frac{v_F \sqrt{n_{2D}}}{\sqrt{\pi}} a_0 \tag{3}$$

In our original paper, we have erroneously computed the Fermi energy ε_F in eq 1 by using the 3D effective electron density n_0^{graphene} instead of the 2D electron density n_{2D}. Since ε_F never explicitly enters the equations but is only a computed quantity, all numerical results and the discussion of the numerical performance of the iterative solution are unaffected. The correct version of Figure 5 is reported in the following Figure 1, while the corrections that need to be applied to the values reported in the original paper are summarized in Table 1.

Table 1. Numerical Values (Old and New) of ε_F, with the Indication of the Associated Graphene-Based System[a]

Position	System	Old ε_F (eV)	New ε_F (eV)
p. 23852, right column	GD20	1.51	0.40
p. 23853, caption of Figure 3	GD20	1.51	0.40
p. 23854, left column	GD20	1.51	0.40
p. 23854, right column	CNTs	1.04	0.19
p. 23855, right column	GDs	1.51	0.40
p. 23856, left column	CNT1M	1.03	0.19
p. 23856, right column	GD1M	1.84	0.60
p. S4, Supporting Information	GD36	1.51	0.40

[a]The same notation as the original text is used. All data are reported in eV.

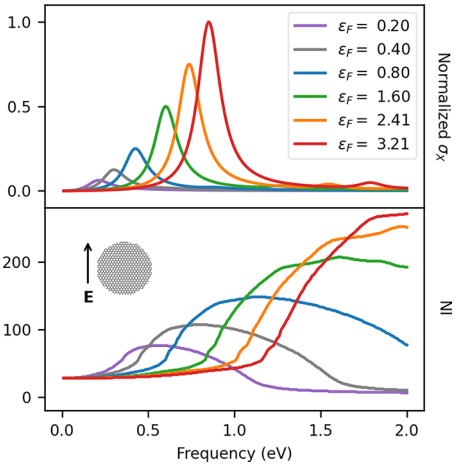

Figure 1. GD20 σ_X (top) and NI (bottom) as a function of the Fermi energy ε_F (given in eV).