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

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In the original paper, the Fermi energy values \( \varepsilon_F \) 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:

\[
\varepsilon_F = \hbar v_F \sqrt{n_{2D}}
\]

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

\[
n_0 = \frac{n_0}{m^*}
\]

where \( n_0 \) 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):

\[
\bar{n}_0 = n_{2D} a_0, \quad m^* = \frac{\sqrt{m_{2D}}}{v_F}
\]

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

\[
n_{0,\text{graphene}} = \frac{v_F \sqrt{n_{2D}}}{\sqrt{\hbar}} a_0
\]

In our original paper, we have erroneously computed the Fermi energy \( \varepsilon_F \) in eq 1 by using the 3D effective electron density \( n_{0,\text{graphene}} \) instead of the 2D electron density \( n_{2D} \). Since \( \varepsilon_F \) 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 \( \varepsilon_F \), with the Indication of the Associated Graphene-Based System

| Position          | System | Old \( \varepsilon_F \) (eV) | New \( \varepsilon_F \) (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                        |

\( \varepsilon_F \) is given in eV.

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

### Figure 1. GD20 \( \sigma_\omega \) (top) and NI (bottom) as a function of the Fermi energy \( \varepsilon_F \) (given in eV).

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