Correction to Organometallic Complexes of Graphene: Toward Atomic Spintronics Using a Graphene Web

[*ACS Nano* **2011,** *5*, 9939–9949. DOI: 10.1021/nn203719a]. Stas M. Avdoshenko,* Ilya N. Ioffe, Gianaurelio Cuniberti, Lothar Dunsch, and Alexey A. Popov*

We would like to correct the errors in the magnetization energy (EM) values listed in Table 1 in our recent paper. The energies used to compute EM values were erroneously taken from the band structure calculations and corresponded to the k-space integration along the high symmetry lines rather than the whole k-space. This resulted in the overestimation of the stability of the spin-polarized states. Corrected values are listed in Table 1. Exchange energies are also affected by this error, and the new set of *J* values is also listed in Table 1. To give a solid estimation of exchange energy per site, the values were computed as the difference of four times the ME value of the system with 1×1 cell size (fully ferromagnetic system) and the ME value of the system with 2×2 cell size and one of the spin flipped ($\uparrow\uparrow\uparrow\downarrow$): $J = 4\mathrm{EM}(\uparrow) - \mathrm{EM}(\uparrow\uparrow\uparrow\downarrow)$. These values show that ferromagnetic coupling is preferable in all cases except for the system I with the shortest Cr−Cr distance. These errors *do not affect* the other results discussed in the original article, including thermodynamic and dynamic stability, band structure, spin density distribution, and local gating of the ligand.

TABLE 1. Relative Energies of Ferromagnetic (spin-polarized) Phase Solutions for Structures I−VIII with Respect to Nonmagnetic (spin-unpolarized) Ones (EM), Magnetic Exchange Energy (*J*)

	I	II	III	VI	V	VI	VII	VIII
EM, meV	6.9	3.8	14.6	18.1	25.3	32.1	16.7	23.1
J, meV	−26.4	1	28.9	20.4	1.4	32.9	17.4	18

Acknowledgment. The authors are thankful to Shulai Lei (Hefei National Laboratory for Physical Science at Microscale) for attracting our attention to the possible errors in the original manuscript.

Published online February 24 2012
10.1021/nn300708n