ADDITIONS AND CORRECTIONS

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Arrigo Calzolari, Rosa Di Felice, Elisa Molinari, and Anna Garbesi: : Electron Channels in Biomolecular Nanowires

Figures 2, 3, and 4 on pages 2511 and 2513 were in error and should be replaced with the following. An incorrect pseudopotential (suffering from ghost states[1] in the factorized form[2]) used to represent the K species gave a fake effect of sp hybridization, with consequent potassium−guanine coupling and p-type doping. We repeated the bandstructure calculations for the G4 wires with a newly generated K pseudopotential,

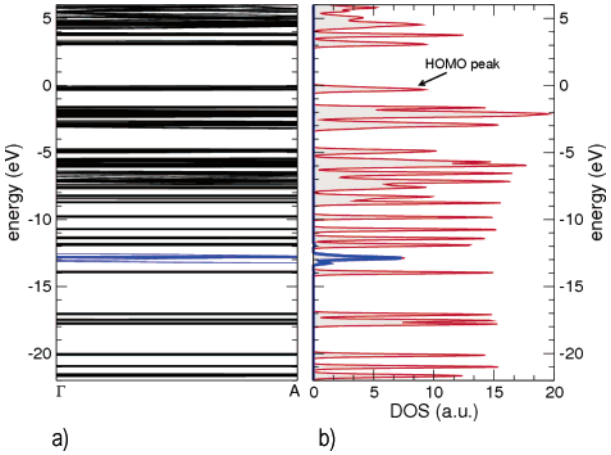

Figure 1. Replacement of Figure 2 on page 2511, Volume 108B. (a) Band structure along the GA direction parallel to the axis of the 3G4/K^+ wire. (b) Total (shaded gray ares), guanine-projected (red line), and potassium-projected (blue line) DOS. A wide energy range is plotted here to show the low-energy peak due to the inner-channel metal.

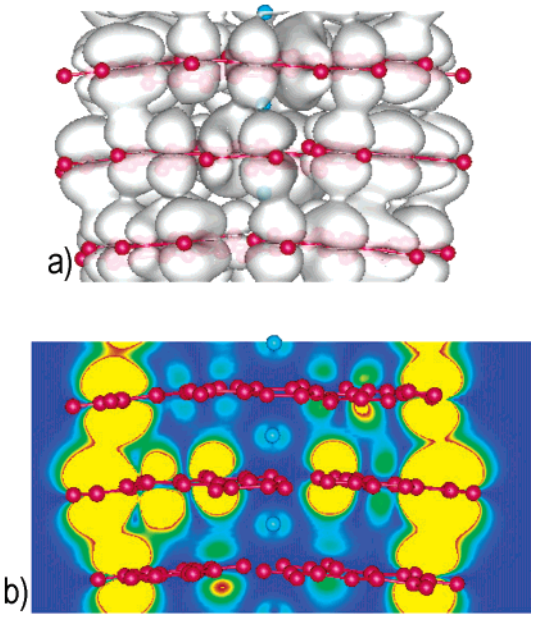

Figure 2. Replacement of Figure 3 on page 2513, Volume 108B. (a) Isosurface plot of the convolution of electron states in the HOMO manifold. (b) Contour plot of the same HOMO convolution, in a K^+-containing plane perpendicular to the tetrameric planes.

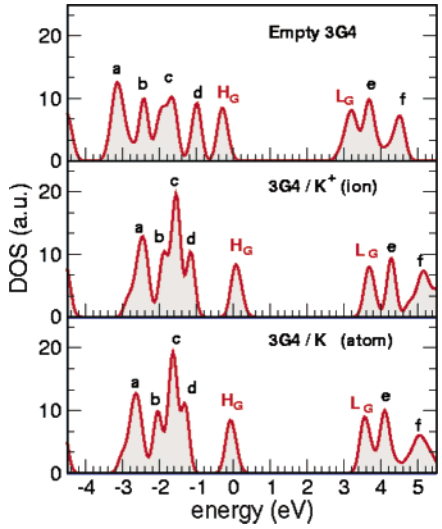

Figure 3. Replacement of Figure 4 on page 2513, Volume 108B. Panels and peaks are labeled consistently with figure caption in the original paper. The HOMO−LUMO DFT energy gap is 3.1 eV for the empty G4 wire and 3.3 eV for the K and K^+ containing G4 wires. The LUMO peak is partially occupied in the 3G4/K system (bottom panel).

containing the 4s and 3p shells explicitly in the valence; both the atomic and bulk bandstructure calculations gave the correct separation (16.5 eV from the all-electron atom) between these shells. We used the PW91 parametrization[3] for the exchange-correlation functional in the supramolecular (G4, 3G4/K, 3G4/K^+, see labeling in the original paper) simulations and consistently generated pseudopotentials for all the species.

We summarize the differences with the previously proposed interpretation. (i) sp hybridization does not occur because the 3p and 4s shells remain well separated in energy. (ii) The manifold-based picture of an effective semiconductor remains valid, but without intrinsic doping; the highest-occupied orbitals of 3G4/K^+ have complete filling and guanine character. (iii) The K 3p orbitals originate a 9-fold peak (the blue peak in Figure 1 stems from 9 electron states coming from the 3p orbitals for each K center in the supercell) at low energy in the projected density of states (PDOS), 13 eV below the HOMO. Their coupling with the guanines is negligible. The K-derived peak is accommodated in a gap in the G PDOS. (iv) The orbital channel for charge motion along the helix goes only through the guanines (see Figure 2). (v) The structure of the occupied portion of the DOS is practically identical for the systems 3G4/K^+ and 3G4/K (Figure 3), the only significant difference being a fractional occupation of the LUMO peak for the latter.

Acknowledgment. We are grateful to Jose M. Soler for pointing out and discussing an inconsistency in the published density of states that allowed us to repair the calculations.

References and Notes

(1) (a) Gonze, X.; Stumpf, R.; Scheffler, M. *Phys. Rev. B* **1991**, *44*, 8503. (b) Gonze, X.; Kickell, P.; Scheffler, M. *Phys. Rev. B* **1990**, *41*, 12264.
(2) Kleinman, L.; Bylander, D. M. *Phys. Rev. Lett.* **1982**, *48*, 1425.
(3) Perdew, J. P.; Chevary, J. A.; Vosko, S. H.; Jackson, K. A.; Pederson, M. R.; Singh, D. J.; Fiolhais, C. *Phys. Rev. B* **1992**, *46*, 6671.
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