Erratum: When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors [Phys. Rev. B 79, 201205 (2009)]

T. Körzdörfer, S. Kümmel, N. Marom, and L. Kronik

(Received 10 September 2010; published 28 September 2010)

DOI: 10.1103/PhysRevB.82.129903 PACS number(s): 61.46.−w, 33.60.+q, 31.15.es, 99.10.Cd

We made a mistake in our paper in the numerical evaluation of Eq. 2 when calculating the data that Fig. 4 of our paper was based on: we used $v_c^{\mathrm{LSDA}}[|\varphi_i|^2,|\varphi_i|^2]$ instead of $v_c^{\mathrm{LSDA}}[|\varphi_i|^2,0]$. Below is a corrected version of Fig. 4 using $v_c^{\mathrm{LSDA}}[|\varphi_i|^2,0]$. As one can see the resulting changes are small. This correction does not alter any of the conclusions drawn in the paper.

We would further like to clarify that the prefactor 0.94 in front of the integral on the right-hand side of Eq. 2 is in our case to be read in Rydberg units, i.e., compared to Eq. 41 of Ref. 1 we included an empirical factor of 0.5.

We thank F. Rissner for checking Eq. 2.

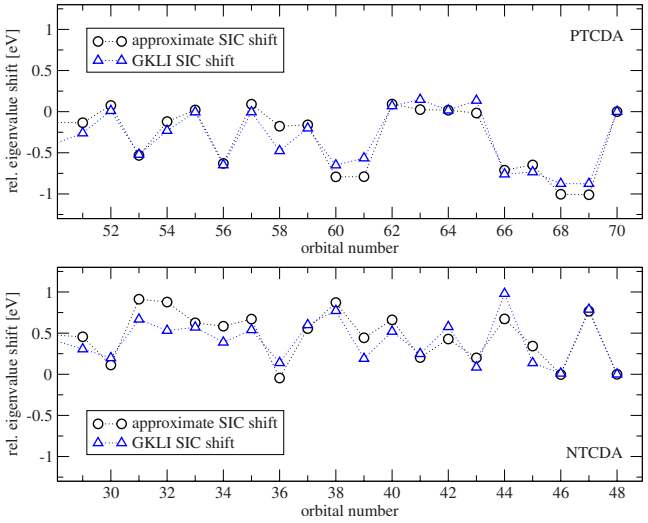

FIG. 4. (Color online) Orbital shift relative to the shift for the HOMO as obtained from the GKLI calculation (blue triangles) and the correctly evaluated Eq. 2 (black circles) for PTCDA (top) and NTCDA (bottom).

[1] J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).

