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Correction to A Finite-Field Approach for *GW* Calculations beyond the Random Phase Approximation

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In ref 1, a coding error led to inaccuracies in the calculation of *GW* quasiparticle (QP) energies evaluated beyond the random phase approximation (RPA). After correcting the implementation, the conclusions of our original contribution remain valid.

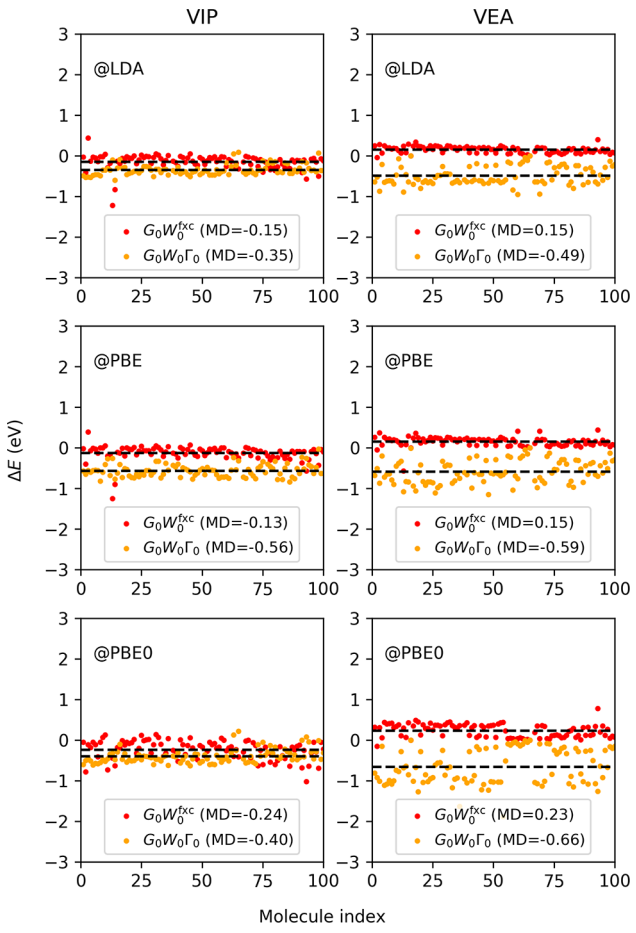

Figure 5. Difference (ΔE) between vertical ionization potential (VIP) and vertical electron affinity (VEA) of molecules in the GW100 set computed at the $G_0W_0^{f_{xc}}/G_0W_0\Gamma_0$ level and corresponding $G_0W_0^{RPA}$ results. Mean deviations (MDs) in electronvolts are shown in brackets and represented with black dashed lines. Results are presented for three different functionals (LDA, PBE, and PBE0) in the top, middle, and bottom panel, respectively.

Here we report updated Figures 5−7 and Tables 1 and 2. The major difference between the updated results and the original ones was found for the quasiparticle (QP) energies of molecules computed at the $G_0W_0^{f_{xc}}$ level. In Figure 5 we show the mean deviation (MD) of $G_0W_0^{f_{xc}}$ and $G_0W_0\Gamma_0$ results from $G_0W_0^{RPA}$ results. The MD between $G_0W_0^{f_{xc}}$ and $G_0W_0^{RPA}$ is −0.15/-0.13/-0.24 eV for the vertical ionization potential (VIP) and 0.15/0.15/0.23 eV for the vertical electron affinity (VEA) with the LDA/PBE/DDH functional, respectively (in ref 1. the MD was 0.30/0.31/0.58 eV for VIP and −0.01/-0.01/0.01 eV for VEA). Although the updated MD values are different from those of ref 1, this difference does not affect our original conclusions, i.e., that the effect of vertex correction at the $G_0W_0^{f_{xc}}$ level is less significant than that found at the $G_0W_0\Gamma_0$ level. We found that the MD between $G_0W_0\Gamma_0$ and $G_0W_0^{RPA}$ results is −0.35/-0.56/-0.40 eV for VIP and −0.49/-0.59/-0.66 eV for VEA with the LDA/PBE/DDH functional, respectively (in ref 1. the MD was −0.74/-0.76/-1.25 eV for VIP and −0.26/-0.30/-0.32 eV). The trend that both VIP and VEA obtained at the $G_0W_0\Gamma_0$ level are lower than those obtained at the $G_0W_0^{RPA}$ level is the same as that reported in ref 1.

For solids, the updated band gap values (Table 2) are similar to those in ref 1, with the mean absolute deviation (MAD) between current and previous results being 0.17 eV for $G_0W_0^{f_{xc}}$ calculations (fifth column) and 0.06 eV for $G_0W_0\Gamma_0$ calculations (sixth column). The largest difference was found in the case of $G_0W_0^{f_{xc}}$ calculations of WO_3 and Si_3N_4, where the updated results are ∼0.3 eV lower than previous ones. The conclusion that in solids the effect of vertex corrections is much smaller than in molecules remains the same.

We emphasize that while the specific numbers reported in the updated tables and figures are different from the corresponding ones in ref 1, the trends observed here are the same as those reported previously and therefore the major conclusions of ref 1

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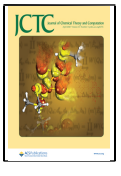

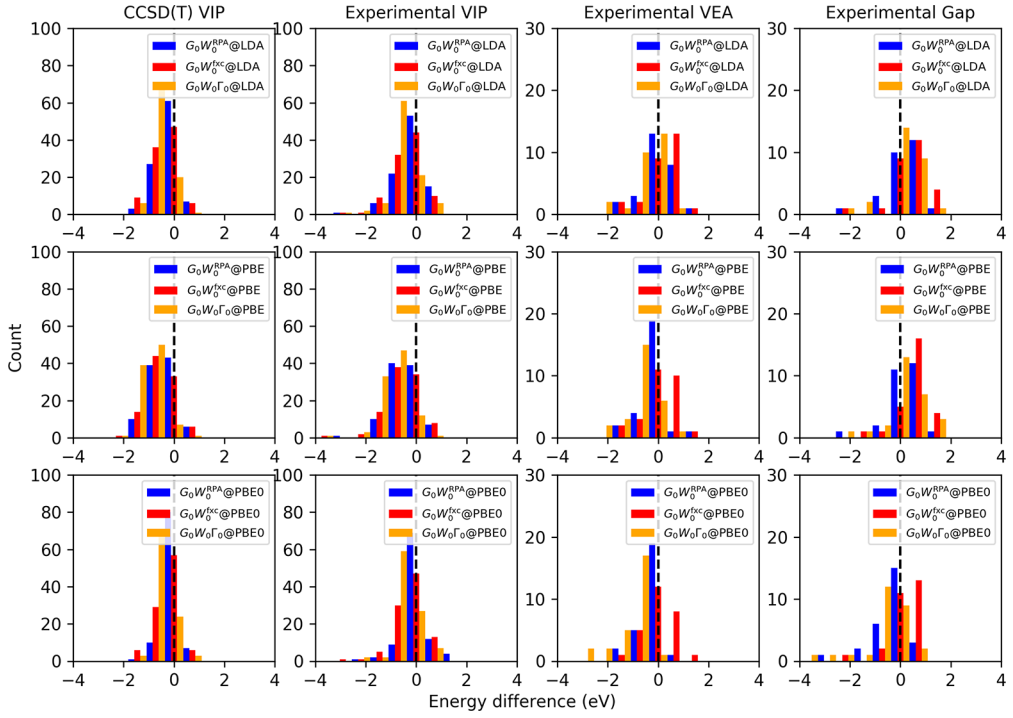

Figure 6. Vertical ionization potential (VIP), vertical electron affinity (VEA) and electronic gap of molecules in the GW100 set computed at $G_0W_0^{RPA}$, $G_0W_0^{f_{xc}}$, and $G_0W_0\Gamma_0$ levels of theory, compared to experimental and CCSD(T) results (black dashed lines).

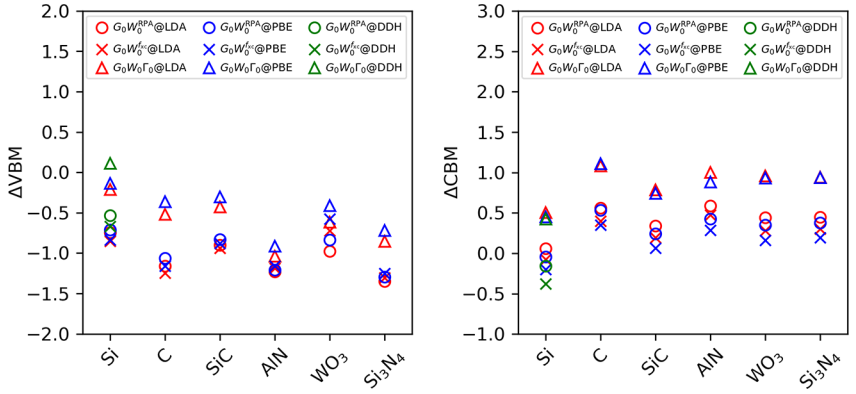

Figure 7. *GW* quasiparticle corrections to the valence band maximum (VBM) and the conduction band minimum (CBM). Circles, squares, and triangles are $G_0W_0^{RPA}$, $G_0W_0^{f_{xc}}$, and $G_0W_0\Gamma_0$ results, respectively; red, blue, and green markers correspond to calculations with LDA, PBE, and DDH functionals.

Table 1. Mean Deviation and Mean Absolute Deviation (in Brackets) for *GW* Results Compared to Experimental Results and CCSD(T) Calculations[a]

	CCSD(T) VIP	exp VIP	exp VEA	exp gap
$G_0W_0^{RPA}$@LDA	−0.23 (0.34)	−0.19 (0.43)	0.04 (0.45)	0.21 (0.56)
$G_0W_0^{f_{xc}}$@LDA	−0.39 (0.48)	−0.35 (0.53)	0.21 (0.51)	0.50 (0.69)
$G_0W_0\Gamma_0$@LDA	−0.58 (0.62)	−0.54 (0.63)	−0.49 (0.59)	0.04 (0.53)
$G_0W_0^{RPA}$@PBE	−0.43 (0.50)	−0.39 (0.55)	−0.09 (0.46)	0.28 (0.57)
$G_0W_0^{f_{xc}}$@PBE	−0.56 (0.62)	−0.52 (0.65)	0.08 (0.49)	0.56 (0.75)
$G_0W_0\Gamma_0$@PBE	−0.99 (1.01)	−0.95 (0.98)	−0.77 (0.84)	0.15 (0.58)
$G_0W_0^{RPA}$@PBE0	−0.05 (0.20)	−0.01 (0.34)	−0.26 (0.41)	−0.26 (0.47)
$G_0W_0^{f_{xc}}$@PBE0	−0.29 (0.39)	−0.25 (0.48)	0.04 (0.43)	0.26 (0.52)
$G_0W_0\Gamma_0$@PBE0	−0.45 (0.49)	−0.41 (0.54)	−1.10 (1.11)	−0.68 (0.75)

[a]We report vertical ionization potentials (VIP), vertical electron affinities (VEA), and the fundamental electronic gaps. All values are given in electronvolts.

remain unaltered. All of the equations in ref 1 remain unchanged.

Finally, we note that the update discussed here does not involve changes to the implementation of the finite-field

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Table 2. Band Gaps (eV) for Solids Computed by Different *GW* Approximations and Exchange-Correlation (XC) Functionals (See Text)[a]

system	XC	DFT	$G_0W_0^{RPA}$	$G_0W_0^{f_{xc}}$	$G_0W_0\Gamma_0$
Si	LDA	0.55	1.35	1.32	1.26
	PBE	0.73	1.39	1.36	1.31
	DDH	1.19	1.57	1.48	1.51
C	LDA	4.28	5.99	5.92	5.88
	PBE	4.46	6.05	5.97	5.93
SiC (4H)	LDA	2.03	3.27	3.16	3.24
	PBE	2.21	3.28	3.15	3.25
AlN	LDA	3.85	5.67	5.51	5.89
	PBE	4.04	5.67	5.48	5.83
WO_3 (monoclinic)	LDA	1.68	3.10	2.69	3.26
	PBE	1.78	2.97	2.52	3.13
Si_3N_4 (amorphous)	LDA	3.04	4.84	4.65	4.83
	PBE	3.19	4.87	4.64	4.84

[a]All calculations are performed at the Γ-point of supercells with 64−96 atoms (see section 1 of the Supporting Information for details).

algorithm presented in ref 1 for the calculation of response functions and exchange−correlation kernels. Therefore subsequent works of ref 1 that deploy the finite-field algorithm and its original implementation (e.g., ref 2) remain unaltered.

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