ERRATA

Erratum: Physical interpretation and assessment of the Coulomb-hole and screened-exchange approximation for molecules
[Phys. Rev. A 40, 4837 (1989)]

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Several errors have been discovered. With one exception, all of these are rather minor. The one exception is that the COHSEX2, M-COHSEX2, $GW2$, and $GW2$ gap properties reported were all inadvertently calculated neglecting a factor of 2. Fortunately, this is rather easy to correct. The COHSEX2, M-COHSEX2, $GW2$, and $GW2$ gap ionization potentials (I) should be corrected using the formula

$$I^{\mathrm{corr}} = I^{\mathrm{SCF}} + 2(I - I^{\mathrm{SCF}}) , \tag{E1}$$

the spectroscopic factors (S) should be corrected using the formula

$$S^{\mathrm{corr}} = \frac{S}{2-S} , \tag{E2}$$

while the spherically averaged momentum distributions [$\Pi(p)$] can be corrected approximately by

$$\Pi^{\mathrm{corr}}(p) \approx \Pi^{\mathrm{SCF}}(p) + 2[\Pi(p) - \Pi^{\mathrm{SCF}}(p)] . \tag{E3}$$

Here the superscript SCF refers to the frozen orbital (Koopmans's theorem) quantity, the superscript corr refers to the corrected quantity, while the absence of a superscript denotes the value appearing in the original paper.

Note that the purpose of this paper was "to define the limits of the COHSEX approximation." The primary conclusions about the relative quality of the COHSEX2, M-COHSEX2, and $GW2$ approximations remain unchanged, but the (corrected) $GW2$ approximation gives results which are similar to the $GF2$ approximation.

Minor corrections are as follows: the $3\sigma_u$ orbitals of F_2 in Table III should be a $3\sigma_g$ orbital, the $1\pi_g$ orbital of C_2H_2 in Table IV should be a $1\pi_u$ orbital, and the Koopmans's ionization potential of the $3a_g$ orbital of N_2H_2 appearing in Table IV should be 18.17 eV (instead of 17.18 eV). The H_2O_2 calculations employed a dihedral angle of 124.7° (contrary to Table I in the original paper). The (corrected) results change slightly when a dihedral angle of 111.5° (original Table I) is used. The SCF total energy becomes -150.5535 a.u. and the dipole moment becomes 2.4591 D (compare Table II). Table I of this erratum corrects the H_2O_2 entry of Table IV in the original paper. A caret should appear over the Fock operator F just after Eq. (2.3), and the left square bracket in Eq. (3.7) should be replaced with a left parenthesis in accordance with the usual custom when a distinction is made between functions and functionals.

TABLE I. Hydrogen peroxide Green-function ionization potentials recalculated with the dihedral angle 111.5°. The experimental ionization potential is the same as in Table IV of the original paper.

Orbital	Expt.	GF2	GW2	M-COHSEX2	COHSEX2	Koopmans's
H_2O_2						
$4b$	11.69	9.75	8.98	8.72	9.96	13.50
$5a$	12.69	11.19	10.77	10.32	12.04	14.25
$4a$	15.33	13.94	13.88	13.29	15.81	16.27
$3b$	17.40	15.65	14.92	14.30	16.71	19.39[a]
$3a$	17.40	16.42	16.13	15.43	18.08	19.18[a]

[a]Order reversal.