# Erratum: Optical Spectrum of $MoS_2$: Many-Body Effects and Diversity of Exciton States [Phys. Rev. Lett. 111, 216805 (2013)]

Diana Y. Qiu, Felipe H. da Jornada, and Steven G. Louie

(Received 3 August 2015; published 9 September 2015)

DOI: 10.1103/PhysRevLett.115.119901 PACS numbers: 73.22.-f, 71.35.-y, 78.67.-n, 99.10.Cd

After further convergence tests, we find that finer $k$ grids than the $12 \times 12 \times 1$ $k$ grid for the dielectric matrix and the $72 \times 72 \times 1$ $k$ grid for the BSE Hamiltonian reported in our Letter are required to converge the calculation. We have increased $k$-point sampling for the calculation of quasiparticle energies to $24 \times 24 \times 1$ and the calculation of the optical spectrum to $300 \times 300 \times 1$. We find that the quasiparticle gap decreases to 2.7 eV and the binding energy of the lowest excitation energy $A$ exciton decreases to 0.65 eV. The main conclusions of our Letter—that $MoS_2$ has a large number of exciton states with large binding energies and the analysis of the character of these states—remain unchanged, but the oscillator strengths of excited states of the $A$ and $B$ excitons in the optical spectrum have decreased, resulting in better agreement with experiment for higher energy states. The $300 \times 300 \times 1$ sampling in our corrected calculation was achieved by explicitly calculating matrix elements on a $24 \times 24 \times 1$ $k$ grid for all transitions in the Brillouin zone and a $300 \times 300 \times 1$ $k$ grid for all transitions where the scattering momentum is less than 0.1 $\text{bohr}^{-1}$. These explicitly calculated

TABLE I. Values from different studies: optical transition energies for peaks $A$, $B$, $A'$, $B'$, and $C$, the binding energy of peak $A$ ($E_b$) and the convergence parameters—$k$-point sampling and number of valence ($N_v$) and conduction ($N_c$) bands. Low temperature experimental results were taken at 10 K [1] and 4 K [2].

| | Optical transition energies (eV) | | | | | | Convergence parameters | | |
|---|---|---|---|---|---|---|---|---|---|
| | $A$ | $B$ | $A'$ | $B'$ | $C$ | $E_b$ | $k$ grid | $N_v$ | $N_c$ |
| Present work ($G_0W_0$) at 0 K | 2.04 | 2.17 | 2.32 | 2.45 | 2.73 | 0.63 | $300 \times 300 \times 1$ | 4 | 4 |
| Present work ($G_0W_0$) at 300 K | 1.96 | 2.09 | 2.24 | 2.37 | 2.69 | 0.63 | $300 \times 300 \times 1$ | 4 | 4 |
| Absorp. exp. at low $T$ | 1.92–1.94 [1,2] | 2.08 [1] | | | | | | | |
| Absorp. exp. at 300 K | 1.88 [3] | 2.03 [3] | | | | | | | |
| PL exp. at 300 K | 1.85 [4] | 1.98 [4] | | | | | | | |
| $G_0W_0$-BSE [5] | 1.78 | 1.96 | | | | 1.04 | $6 \times 6 \times 1$ | 2 | 4 |
| sc-$GW$-BSE [6][a] | 2.22 | 2.22 | 2.5 | 2.5 | | 0.63 | $15 \times 15 \times 1$ | 6 | 8 |

[a]Spin orbit was not included in this calculation.

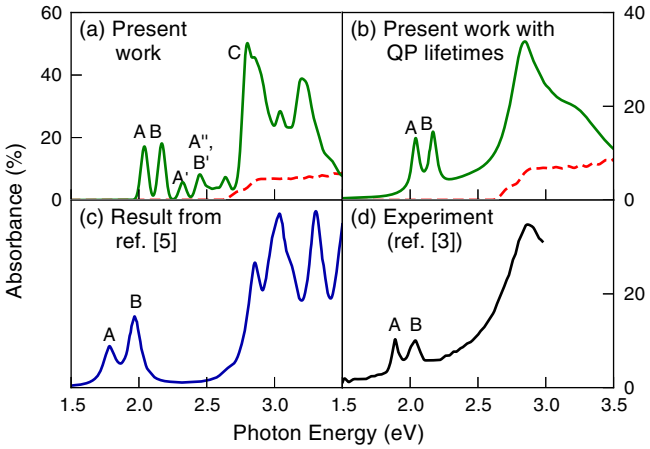


FIG. 1 (color online). (a) Absorption spectra of $MoS_2$ without (dashed red curve) and with (solid green curve) electron-hole interactions using a constant broadening of 25 meV. (b) Same calculated data as in (a) but using an *ab initio* broadening based on the electron-phonon interactions [7,8]. (c) Previous $G_0W_0$ plus BSE calculation (in arbitrary units) [5]. (d) Experimental absorbance [3].

 

matrix elements are interpolated to all points on a uniform $300 \times 300 \times 1$ $k$ grid. This fine sampling is necessary to capture fast variations in screening at small wave vectors and fine features in the exciton wave functions, which are tightly localized in $k$ space.

We have summarized the corrected quantitative results in Table I, which replaces Table II on page 3 of our Letter. In the table, we have added the effect of lattice expansion due to temperature to draw a more accurate comparison with experimental measurements taken at room temperature, as noted by Soklaski *et al.* [2]. Figure 1 replaces Fig. 2 on page 3 of our Letter.

We thank Dr. Li Yang and Dr. Junichiro Kono for bringing the issue of temperature effects to our attention.

[1] K. F. Mak, K. He, C. Lee, G. H. Lee, J. Hone, T. F. Heinz, and J. Shan, Nat. Mater. **12**, 207 (2013).
[2] R. Soklaski, Y. Liang, C. Zhang, H. Wang, F. Rana, and L. Yang, Appl. Phys. Lett. **104**, 193110 (2014).
[3] K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, Phys. Rev. Lett. **105**, 136805 (2010).
[4] A. Splendiani, L. Sun, Y. Zhang, T. Li, J. Kim, C.-Y. Chim, G. Galli, and F. Wang, Nano Lett. **10**, 1271 (2010).
[5] A. Ramasubramaniam, Phys. Rev. B **86**, 115409 (2012).
[6] H. Shi, H. Pan, Y.-W. Zhang, and B. I. Yakobson, Phys. Rev. B **87**, 155304 (2013).
[7] A. Marini, Phys. Rev. Lett. **101**, 106405 (2008).
[8] X. Li, J. T. Mullen, Z. Jin, K. M. Borysenko, M. Buongiorno Nardelli, and K. W. Kim, Phys. Rev. B **87**, 115418 (2013).