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Erratum: Molecular oxygen tetramer $(O_2)_4$: Intermolecular interactions and implications for the ϵ solid phase [Phys. Rev. B 84, 092105 (2011)]

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We have found a mistake in Fig. 3. In the text of the article it is stated that, for obtaining the optimized intra- and intercluster distances d_m and D_m, a *spin-averaged* $(O_2)_2$ potential has been employed for the V_{ij}^{inter} pair potential between molecules i and j belonging to different clusters. However, the results displayed in the *lower panel* of that figure were erroneously obtained using a *triplet* $(O_2)_2$ potential. The corrected results are shown in the accompanying figure. Please note that the upper panel of Fig. 3 and complementary information (in the text) are correct in the original work.

As can be seen in the amended figure, comparison of the correctly computed distances d_m and D_m with the experimental data is slightly worse in the lower pressure range, but better for the highest pressures. Differences with the previous values are quite small (about 0.05 Å), and the overall behavior is quite similar. This is due to the resemblance between the triplet and the spin-averaged $(O_2)_2$ interaction potentials: since the triplet state energies lie between those of the singlet and quintet states, they are close to the spin-averaged values. Conclusions of the work remain unaltered, specifically, the key role of the repulsive wall of the singlet $(O_2)_4$ interaction potential (obtained at a multiconfigurational level of theory) in the modeling of the structure of the ϵ phase.

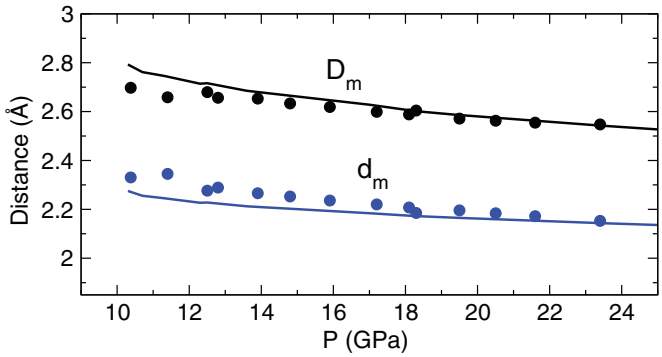

FIG. 3. (Color online) Lower panel: pressure dependence of d_m and D_m (lines) compared with data of Ref. 1 (circles). See text for details.

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