Saito and Oshiyama Reply: In the preceding Comment [1] on our Letter [2], Watkins shows his confidence that large pairing distortion (LPD) takes place instead of the resonant-bond distortion (RBD) in the divacancy (V_2) for both V_2^+ and V_2^-. His assertion is based on the EPR measurement beautifully carried out by Watkins and Corbett in the 1960s [3]: They have established that the pairing distortion is consistent with the EPR spectra under uniaxial stress. We still argue, however, that the RBD occurs for V_2^- and the small pairing distortion occurs for V_2^+, based on our careful total-energy calculations newly performed and on a notion that the RBD is *not* inconsistent with the EPR measurement under uniaxial stress.

In order to reexamine our finding that the pairing distortion is small in the divacancy, we newly perform more careful total-energy calculations within the local density approximation (LDA): We carry out more extensive search for stable geometries and also increase the number of k points in the Brillouin zone integration. Again we obtain the results of a small size of the pairing distortion: The distance (l_{23}) between the pairing atoms is 3.48 Å (3.55 Å in Ref. [2]) for V_2^-; the unoccupied a_g level which splits from the upper e_g level is found to have much higher energy (0.41 eV) than the a_u level, the upper partner of the b_u level split from the e_u level. It is noteworthy, however, that a metastable geometry in which a relatively LPD ($l_{23} = 2.93$ Å) takes place is found when we perform a restricted LDA calculation by enforcing the electron configuration as $b_u^2 a_u^0 a_g^1$. This excited geometry is 0.26 eV higher in total energy than the small pairing geometry and is thus energetically unfavorable. In spite of this large distortion, the a_g level is still located above the a_u level by 0.06 eV. When we render the pairing atoms closer (e.g., $l_{23} = 2.81$ Å), the energetical order of the a_u and a_g levels is reversed. However, we do not find any stable geometry with $b_u^2 a_g^1 a_u^0$. The results here, along with the previous results [2], are indicative that the LDA scheme does not produce the stable geometry accompanied with the LPD in Ref. [3].

What should be addressed then is the compatibility between the RBD and the EPR experiment with uniaxial stress [3]: The stress along the particular axis of ⟨110⟩ induces the total-energy difference among orientations of the defects in a crystal and this energy difference is observed from Boltzmann distribution of the EPR line intensity corresponding to each orientation. It is found from the observation for V_2^+ and V_2^- that the defect in which the stress reduces the distance l_{23} between the nearest two atoms on the pairing axis (this orientation is denoted by *ad* in Ref. [3]) has lower energy than that in which the stress reduces another distance (l_{12} or l_{13}) between two of three neighboring nearest atoms (*ab*). We certainly agree with the notion that the pairing distortion model is consistent with the experimental result (our new calculation on V_2^- actually shows that the defect of *ad* has lower energy by ~0.01 eV than that of *ab*). We do not agree, however, with a notion that the RBD model is inconsistent with the EPR spectra. In this model, the defect of *ad* is likely to increase in total energy by the stress, since the direction of the RBD is opposite to that of the stress. The point is, however, that the total energy in *ab* is also expected to increase. The stress which makes l_{12} small causes disruption of the resonant bonds (two resonant bonds disappear and the remaining one becomes pairinglike). If the increase in the total energy is larger for the latter than for the former, the EPR data under the uniaxial stress is consistent with the RBD model.

In the Jahn-Teller system with two-dimensional e-mode space, the energy barrier in the reaction from one Jahn-Teller distortion direction to another could be much smaller than the Jahn-Teller energy. This was actually observed in transition-metal or ionic compounds. In covalent materials, however, any reaction pathway is accompanied with the bond stretching and bending. We thus suspect that the reaction pathway like the "Mexican hat" really exists in the Jahn-Teller system in the covalent materials.

In conclusion, our careful LDA calculations do not support the LPD for the Si divacancy. We thus believe that the RBD, which naturally explains the character of the wave function observed by the EPR experiment, is suitable for V_2^-. Further theoretical efforts, including energetics under uniaxial stress and calculations of hyperfine tensors and g values, are certainly necessary. Recognizing success of LDA calculations in the past, we believe that the present calculational scheme is capable of describing the properties of the divacancy. Yet we do not exclude a possibility that the new calculational scheme beyond the LDA provides different results. To proceed along this way, further detailed comparison between the LDA results and the experimental data is imperative.

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