

Mutou and Kontani Reply: We thank the authors of the Comment [1] for giving us an opportunity to express our opinion in more detail. We agree that the NaCl-type charge ordering will be favored if only on-site Coulomb interaction U and the nearest-neighbor one V are taken into account. However, we cannot agree with their assertion that V is much smaller than t_0 for the following reasons.

(i) *Concerning (1) of the Comment.* In Ref. [2], it was reported that the charge-ordering state disappears under the chemical pressure. The authors of the Comment agreed that the result is a sign of the irrelevance of V for COO. However, the transfer integral between atoms t_0 should increase in proportion to a^{-7} (a denotes the intersite distance). Thus, V/t_0 decreases when a becomes short. We interpreted the result shown in Fig. 4 of [2] as a consequence of the nonstabilization of COO due to the reduction of U/t_0 and V/t_0 , as we mentioned in [3].

Next we investigate the effect of the long-range Coulomb interaction beyond V because it is important. Interestingly, the energy difference between the CE-type charge ordering and the NaCl-type one is much smaller than V in this case as follows. The long-range Coulomb interaction between i, j -sites with the distance $r_{i,j}$ is given by $V_{i,j} = aV/r_{i,j}$. The potential energy per electron is given by $E_p = \sum_{i,j} V_{i,j}/(2N)$, where i, j run all sites with electrons and N denotes the number of electrons. We calculated the difference ΔE_p between the potential energy for the CE-type charge ordering and that for the NaCl-type one, and found that $\Delta E_p = 0.0668V$. If we take only the nearest-neighbor-site interaction $\{V_{i,j}|r_{i,j} = a\}$ into account, we get $\Delta E_p = V$. Even if we assume Yukawa-type screened interactions, we see that the energy difference rapidly decreases as a screening length ξ increases and it becomes $0.1V$ for $\xi/a \approx 2$. Thus, the energy difference between these two structures of the charge ordering is much smaller than V . Our scenario in [3] is that two-dimensional COO structures are caused by U and V , and then they stack as the CE-type way owing to the gain of the smaller Jahn-Teller (JT) energy. We also consider that the antiferromagnetic correlation between nearest-neighbor sites may assist the CE-type charge ordering to some extent.

(ii) *Concerning (2).* As we pointed out in Ref. [3], we treated the two nonorthogonal orbitals in our simplified model. As for this problem, Khomskii *et al.* have already pointed it out in [4], and they have also performed the mean-field calculation. We are preparing to study on this problem in detail.

(iii) *Concerning (3).* The authors estimated V/t_0 by using the dielectric constant from experiments [5]. However, this is an unreasonable procedure because the dielectric constant is a macroscopic quantity. The value of V/t_0 estimated by the authors is apparently underestimated because there is only one oxygen between nearest-neighbor Mn-ions. (In the Comment, the authors mentioned the esti-

mation of V/t_0 by the calculation of the Madelung energy, and showed the value of $V/t_0 = 0.5$. However, the ratio cannot be determined from our calculation of the electrostatic energy.)

In reality, $V \gtrsim t_0$ is realized in some other transition metal oxides. For example, $V \sim 0.8$ eV was reported by the EELS measurement for Sr_2CuO_3 [6], and the similar value of V was also used in the theoretical study of the optical conductivity [7] and suggested by the EELS measurement for α' - NaV_2O_5 [8]. It is natural to expect the similar situation in Mn oxides. At least, the authors should show the reasonable reason why $V/t_0 \ll 1$ can be realized in the Mn-oxide if they still want to claim that point. Moreover, we would like to suggest that the larger value of V is expected not to destroy the ferromagnetic metallic state observed experimentally because the screened effective repulsive interaction can be smaller in the metallic state.

(iv) *Concerning (4).* We agree that our simplified model may be insufficient to reproduce completely the detailed complex COO pattern observed experimentally. Actually, we wrote in [3], "it is insufficient to ascribe the origin of the stripe structure only to the JT effect." It is a great future problem to treat the system with including both the long-range Coulomb interaction and the JT effect on the same footing. Then, we will know the real mechanism of COO without ambiguity.

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