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Benjamin J. Morgan, David O. Scanlon, Graeme W. Watson
- 069102 Reply to “Comment on ‘Generalized Gradient Approximation +U Study for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide’” (2 pages)**
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In the comment, Morgan et al. reported the calculations for the supercell model using the semicore-hole approximation. They also mentioned that the calculated E_F values were higher than the semiconductor band structures. In the comment, Morgan et al. reported the calculations as closely as possible but they obtained metallic band structures in a metastable state in the supercell calculations. I was not able to determine stable states other than the metallic states. The calculating method and conditions are almost the same as those I used. However, since the calculation code, the pseudopotentials, and the initial states are different from each other, there is no guarantee that the other results are obtained. It is also conceivable that either or both of the results are in metastable states. However, if the result the Morgan et al. obtained is the metastable structure, the disagreement between the calculation result and the experimental result may be due to the difference in the supercell size.

If the result of Morgan et al.² is correct, the properties of Nb-doped TiO₂ cannot be explained by the obtained band structure. We will have to consider the defects or complexes between those defects and atoms in investigate the origin of metallic phases. If the metallic band structure is correct, the result of Morgan et al. might be a metastable state or obtained by inappropriate E_F values. In that case, the calculated E_F values must be appropriate and the semicore-hole structure might be obtained using the E_F . However, to solve this problem completely, we need to establish methods by which the electronic structure is correctly calculated, or perform precise experiments in the stable states in Nb-doped TiO₂.