

## Reply to reviewer 5

We thank the reviewer for his/her careful reading of the manuscript and the insightful comments and suggestions.

- We agree that quantitatively the differences in calculated Fe-O  $\pi$ -bond orders between **1** and **3** are small, however, we want to focus on the trends and have rephrased the sentences accordingly (section 3.5.3., below Table 6).
- The symbol in front of “~ 20,000” has been changed from “<” to a “>” on page 19 ,line 12.
- Yes, the MO phases of interaction in the TOC figure are mistaken, we changed the TOC and Figure 12 according to the suggestions of the reviewer. Thank you!
- We have taken out Table 8 in order to focus and clarify the discussion section, which has also been significantly tightened.
- The misspelling has been corrected.