Atmos. Chem. Phys. Discuss., 11, C4311–C4312, 2011
www.atmos-chem-phys-discuss.net/11/C4311/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Ab initio studies of $O^{-}_{bf2}(H_2O)_{\vec{n}}$ and $O^{-}_{3}(H_2O)_{\vec{n}}$ anionic molecular clusters, $n \leq 12$" *by* N. Bork et al.

Anonymous Referee #2

Received and published: 5 June 2011

The solubilities of anions are still interesting topics to understand better hydrogen bonding interaction and ionic interactions. This study provided the solubility of O2- and O3- in water clusters using an ab initio study. They provided that the excess electron is localized on O2- and O3-. The O2- and O3- reside on the surface of water clusters up to n = 12. The paper is well organized.

Here, I have a few of comments to improve this paper.

1) typo: page 13958, line 18: HOMO orbita —> HOMO orbital.

2) page 13959, if possible, can you provide the table for (R4-R7) as a summary?

3) page 3959, line 23. please check the following correction:

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

O2 clusters —> O2- (H2O)n clusters

O3 clusters —> O3- (H2O)n clusters

4) Personally, Section 3.4 Simple chemistry is understandable, but it seems to me that they discussed the charge transfer will be occurred from O2-(H2O)n to O3 without the strong computational data.

I recommend this manuscript for publication either with or without revision.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 13947, 2011.