SAIP-2019 Reviewers Comments

We would like to thank all reviewers for their insightful comments on this paper, all this comments and suggestions led us to an improvement of the work. Detailed response to reviewers are given below.

Comments Review 1

- It is not mentioned how the U value is obtained chosen. A wrong U value can lead to wrong results. So this needs to be explained.
= U-value parameter of TiO_2 was chosen based on literature, ref. was included

- Which pseudo-potentials have been used. Please always give that information to ensure your results are reproducible.

=Norm conserving was used

- You don't give the thickness of the slab and the inplane size of the unit cell. This is important information to judge whether your simulation set-up is reasonble and yields quantitavily converged results.

=Unit slab size and slab thickness was included on the methodology section

- Please explain how you distinguish/define physisorption and chemisorption

= the difference was captured on section 3.1 (results)

- PBE is known to perform badly for absorption energies. Justify your choice for functional and how accurate the results are expected to be.

= The PBE functional is a widely used function as has been shown to give reliable results in terms of atomization energy and adsorption energy on metal oxides.

-Figure 4 unclear

=This figure focuses on charge redistribution (Ti-F/O-H) during the interaction, however, the charge/iso-surface overlap creating large iso-surfaces. The main aim is to show the depletion and accumulation regions. The calculation was not redo, due to time and calculation constrains. We acknowledge the suggestion and will look to that in future work.

- Mulliken analysis is intrisically a very crude and somewhat unreliable method. A charge transfer of 0.1e is fairly little and within the uncertainity of the method. So not convincing

= Mulliken analysis tend to give qualitative results and the fastest way to calculate atomic charges.

-Grammatical issues

=checked

Comments-Review 2

There is a concern about whether there is enough data in Figure 3 to make a meaningful conclusion. Sentence 2 in the paragraph preceding Fig. 3 reading:

“For all surfaces considered the adsorption energy become more stable with increasing HF coverage” is

matter of fact and should be clarified.

= To increase the data (enough data) one needed big surface slab which is computational intensive. In this study the coverage adsorbate (HF molecule) range from 1-3 HF molecules per each slab surface. In future will work to big systems.