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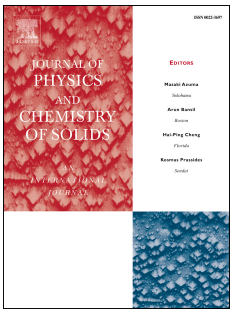

Exploring the sensitivity of nanodiamond to sarafloxacin: A DFT approach

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Reply to the reviewer's comments 25th of June 2018

Firstly, we thank respected editor and reviewers for reviewing the manuscript Number Ref: PCS_2018_557_R1 with the following title:
"Exploring the sensitivity of nanodiamond to sarafloxacin: A DFT approach

This manuscript has been modified according to the reviewer's comments:

-Reviewer 3

Comment: The subject announced in the abstract seems to be interesting. The environmental effect of sarafloxacin is important and it is well described in the introduction. However, the models used and calculations level are not adequate for the objectives of authors in this work, and the conclusions are too weak and not correct. Most of my previous comments for the previous version have not been addressed. Therefore, I think that this manuscript cannot be published in the present form in the Physics and Chemistry of Solids journal. Probably authors can submit it to another journal.

Answer: *Firstly, we would like to thank you for accepting to review our manuscript. Secondly we are apologizing for not receiving our answer sheet to your first series of comments, therefore we will attach the new answer sheet as part of manuscript to be sure that you will receive it.*

Comment 1: The most important conclusion is wrong, the organic did not decrease the HOMO-LUMO gap energy, but the adsorption complex maintains the gap of the sarafloxacin and no improvement is observed.

Answer: *we modified the conclusion of the manuscript." Indeed, the value of HOMO-LUMO gap can influence the other physical properties such as electrical conductivity or resistivity…"*

Comment 2: In Figure 6 the labels or graph lines are wrong.

Answer: *The labels are correct. The arrangements of DOS curves were based on the downward shifts of Fermi levels toward HOMO states in presence of the interaction with antibiotic as explained in manuscript.*

Comment 3: The SIESTA code is useful to use for periodical systems. For molecular clusters, other codes for molecules, such as, Gaussian, Newchem, Gamess, ADF, etc… can be better with better basis sets.

Comment 4: The reasons to choose these calculation parameters, k-points and energy cut-off. Authors should performed preliminary calculations to optimize these parameters.