Dr. Yan Li
Associate Editor
Physical Review B

June 4, 2019

Dear Dr. Li,

Attached is the revised version of our paper entitled *Ab initio modeling of optical functions after strain wave perturbation for defect detection*, manuscript BD13947/Anderson. We hope that we have resolved the very valid point of the first reviewer, and that our manuscript is now acceptable for publication in Physical Review B.

Best regards,

Dr. Sean M. Anderson
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1 Second Report of the First Referee – BD13947/Anderson

In the revised version of the manuscript, the authors have addressed my most important worry about their approach (I am the first referee) by making an explicit connection to the time evolution of the signal in Fig. 4. The new material about the electron density around the defect level is a welcome addition to the manuscript and should help the reader visualize the system. Besides the following minor point, I recommend that the manuscript is accepted for publication in Phys. Rev. B.

Both the second referee and I raised the issue of the different scissors shifts used for surface and bulk susceptibilities. Most importantly, the authors notes in their reply that the exact value used has a negligible influence on the final results. However, they have not modified the manuscript to explain better the values used (except to clarify that 3.4eV is the experimental "direct" optical gap, as I requested, corresponding to the E1 critical point in the JDOS), and any reader with familiarity with DFT calculations of silicon would have a reaction similar to ours. Having looked at the references cited by Referee 2, as well as the authors' previous publications on the system, I have to say I cannot remotely understand where they obtain the value of 0.98 eV for bulk Si from. To quote:

"a scissors shift of 0.98 eV was used for the bulk calculation in order to adjust the theoretical band gap to the experimental value of 3.4 eV for the direct band gap."

This implies the position of E1 in their DFT-LDA calculation was 2.4eV. This is far lower than any calculation I have seen in the literature. Or to put things differently, a bulk Si GW calculation yields shifts ranging from 0.7eV (Botti PRB 10.1103/PhysRevB.69.155112) to 0.95eV (Adolph PRB 10.1103/PhysRevB.53.9797). This yields spectra that overshoot the experimental spectra by a significant amount: hence Schmidt (PRB 10.1103/PhysRevB.61.7604) uses a 0.5eV shift to match with experiment, as the second referee notes. Li (Ref 59) even state "Self-energy corrections to surface states are larger in magnitude by 0.2–0.3 eV than those to bulk states in the same energy range", which would imply the bulk correction is smaller, not larger, than the surface correction of 0.7eV.

Last, it is anyway odd/inconsistent to use a GW-computed value for the surface, and an empirical value for the bulk.

I, therefore, urge the authors to rectify this matter, either in a resubmitted version or a footnote added at the proof stage. It does NOT preclude acceptance in Phys Rev. B, but in my opinion, it looks like an error that can easily be corrected.

Thank you for your shrewd and accurate remarks concerning our values for the scissors shift.

We are in complete agreement that there is no justifiable reason to use a different value for the bulk. Therefore, we have recalculated every result presented in the manuscript using the same 0.7 eV value for both surface and bulk susceptibilities. We have amended the phrase on page 3 (red text) to reflect this change.

The trends of these new results (and our original conclusions), remain the same as in the previous version of the manuscript; however, there are some minor changes to Figs. 2–4 (in the new version of the manuscript) that reflect the new numerical values.

We hope that with these corrections you can recommend acceptance in Phys. Rev. B.