Supplemental Material: Effect of strain and many-body corrections on the band inversions and topology of bismuth

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We here present some more data which may be of interest to the reader. In particular we plot the fitted values for the internal displacement and show how it affects the main features of the electronic structure. The LDA results are also shown for comparison with the GGA. Furthermore, the remaining G_0W_0 results for the overlap are included for completeness. Finally, the band structures of the expanded cells in Fig. 2 of the main text are provided in a separate file.

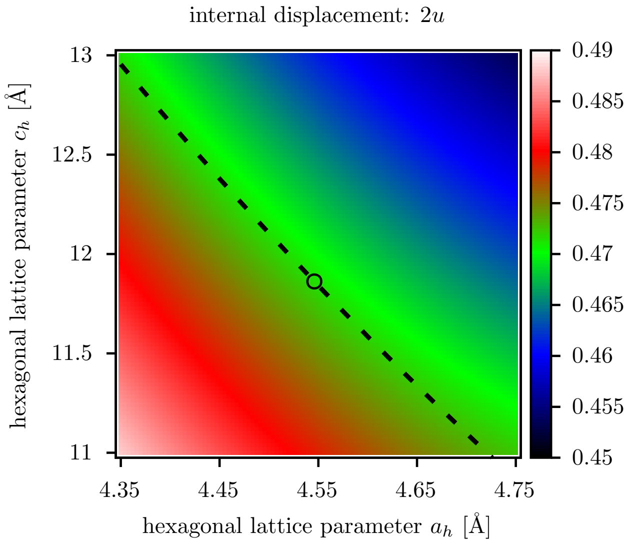

Figure 1. Plot of the internal displacement as a function of the hexagonal lattice parameters a_h and c_h. We show the value of $2u$, i.e. the smallest distance between the two basis atoms along the trigonal axis. For $2u = 0.5$ there is no displacement of the atom from the middle of the cell. As we can see, under the assumption of constant volume, keeping u fixed is a good assumption.

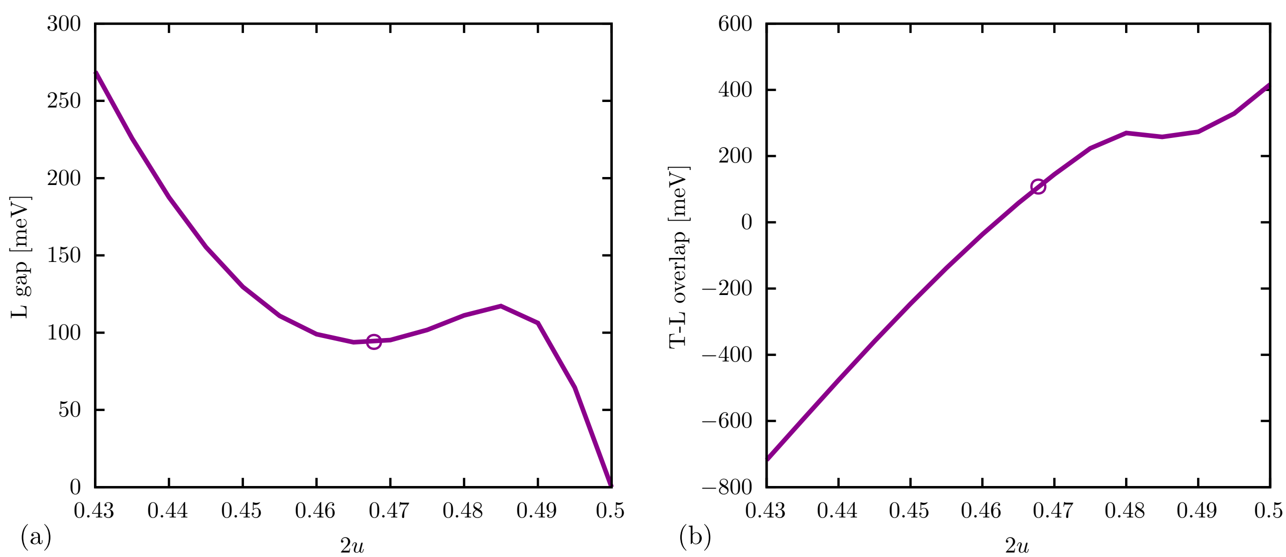

Figure 2. The effect of the internal displacement on (a) the L gap and (b) the indirect T-L overlap is shown. The results for the experimental displacement of $2u = 0.46778$ are highlighted with a circle. The remaining two cell parameters a_r and α were not changed and we used their literature values for all calculations. We find that the optimized $2u = 0.47131$ is close to the experimental value and the minimum L gap and that a small variation, e.g. due to imperfect relaxation, is likely to increase the gap but otherwise does not have dramatic effects. The overlap on the other hand changes more dramatically. Approaching $2u = 0.5$ brings the structure closer to the cubic limit (although still $\alpha \neq 60^{\circ}$) and the L gap vanishes completely.

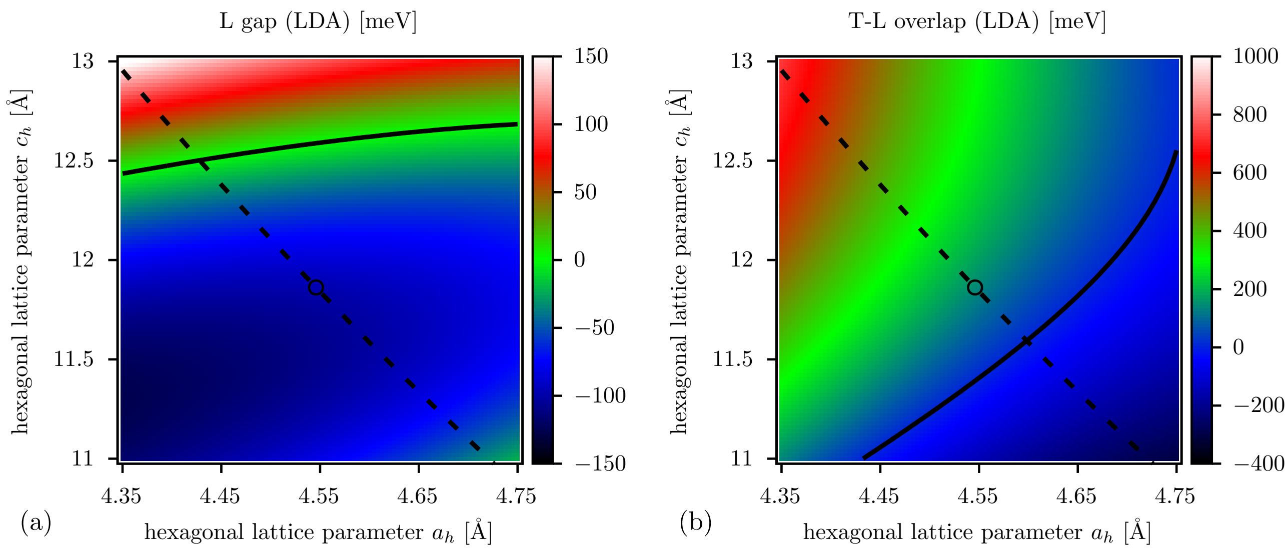

Figure 3. LDA results for the L gap and T-L overlap. There is no significant qualitative difference to the GGA.

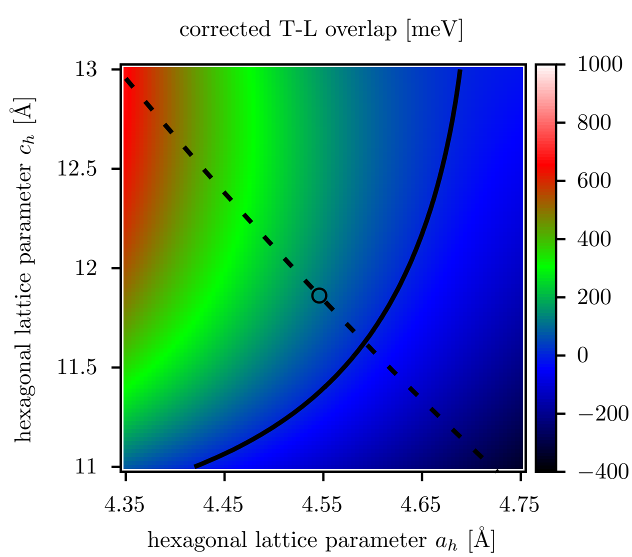

Figure 4. Plot of the indirect overlap with G_0W_0 corrections.