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REPLY TO COMMENT

Extracting convergent surface formation energies from slab calculations

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Abstract. We reply to the preceding comment by Boettger and coworkers.

We are pleased that our numerical confirmation [1] of Boettger's observation [2] is deemed correct [3]. As we discussed in our paper, we think that the solution of taking a linear fit to the slab (or ordered film) energies is obvious. Correspondingly, we are not surprised that this had already been suggested by Gay *et al* in an extended abstract of 1983 [4]. We point out, however, that [4], while suggesting the linear fitting idea, neither includes any analysis of the $\sigma(N)$ behaviour, nor does it compare the results with other methods, nor indeed does it solve the divergence problem, because the problem was simply not known at the time.

As the comment [3] points out, the new and original contribution of our paper is that the linear divergence, be it ever so small, must *always* swamp out meaningful results as slabs become thicker. Boettger's calculations generally employ a different procedure to handle the bulk and slab systems, using either a different basis set [5] or in some cases a different method [2]. Modern *ab-initio* approaches such as FLAPW, FP-LMTO, or pseudopotentials-plane waves, on the other hand, take care to use exactly the same basis set for both systems. Workers using these methods thus generally assume that Boettger's observations, while interesting, do not concern them in practice. Our principal aim was to check this assumption, using in particular the FP-LMTO method. The unexpected outcome was that for moderate slab thicknesses, the linear divergence can lead to non-negligible errors. We consider this numerical result of interest to others, without claiming priority for all the underlying ideas, and regret if this was not made clear enough in our paper.

References

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