Despite our recent article[1], which very clearly outlined how our gas-phase EVB surface was for all intents and purposes faked in Ref. [2] (presumably in order to cover up problems with the authors' adaptation of our EVB), it has recently been brought to our attention that the authors are claiming that *we* faked *our own* results. Now, despite the fact that such a claim is completely ludicrous (as, amongst other things, if it were indeed the case, we would have had nothing to gain from making our data available online here on the web page), we will try to re-clarify a few basic points (which were already clarified in Ref. [1]):

1. The authors of Ref. [2] claimed that the gas-phase surface that was generated by *our* EVB code (as implemented in our MOLARIS software package) is incorrect. The problem with this claim is the fact that the authors never actually used our code. That is, the incorrect surface presented in Ref. [2] was generated using the authors' own adaptation of our EVB code, a point which is not made clear to the readers of Ref. [2]. Now, while we have provided enough information in our existing EVB papers for our code to in principle be reproducible, as anyone who works with method development knows, all sorts of errors can occur when attempting to re-implement someone else's code. Therefore, it is *crucial* to compare any new code to the original implementation, *particularly* if the results being obtained diverge from one another (as such differences usually arise from an incorrect implementation of the original code). Had the authors unsuccessfully attempted to reproduce the results of a major molecular simulation package such as CHARMM, AMBER or GAUSSIAN without direct comparison to the original code, provided poor results in a high profile article, and then provided this as evidence of the inaccuracy of the original code, neither the developers of the original program nor the scientific community at large would stand for it. Yet that is precisely what is happening here, and we consider this to be extremely unprofessional.

2. Following on from point one, we have already clarified both in Ref. [1], and on the website, that the actual results obtained by running our EVB code as implemented in MOLARIS are completely different to those presented in Ref. [2], which we have demonstrated by providing the correct results and a limited access version of the original program here on our website. We will leave the reader to make the final judgment as to what motive could have lain behind the authors of Ref. [2] publishing entirely incorrect results, without ever comparing to our code (or in any way consulting us about the discrepancy in the results), and using this as evidence of the poor performance of our program.

Now, in view of the circumstances, we believe that we have been both gracious and restrained in our response, merely clarifying the fallacies of the arguments against our EVB approach as presented in Ref. [2], and providing the reader with the correct results, leaving the final

judgment to the reader. Despite this, however, the authors of Ref. [2] appear to be still insinuating that we have faked our own results as they cannot reproduce our surface. This despite the fact that we cannot tell our MOLARIS simulation package (which is available to the reader for instant download in a limited version on this part of our website and a full version upon request) what data to produce, and this is the same simulation package that was used to generate the results of both our earlier work[3, 4] and current work[1]. It has reproduced the solution results from our 2004 paper consistently, and we are now also presenting the gas-phase surface, which was not provided in our previous work, as it was not directly relevant to the issue being studied there. However, in the very unlikely scenario that there is concern that we have somehow "implanted" the relevant results into the program, we are also now adding the actual *code* of the relevant part of the program so that someone who would like to write a small EVB program can in principle reproduce the energy at the relevant points. We do this knowing that it will not stop anyone with ill intent from trying to mislead the scientific community at large, but hope that the evidence presented here will be sufficient for any unbiased reader. We would also like to point out that we provided one of the authors of Ref. [2] with a functioning executable in 2003, and had they used this they would have quickly obtained the correct results.

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