

Smith, Hong, and Srolovitz Reply: The 78% Harris [1] functional (HF) error for the Al(111) surface energy reported in Refs. [2,3] is an order of magnitude larger than HF errors typically reported for other calculations of bulk, surface, or molecular energies, as summarized in Table I.

This prompted us [6] to carry out extensive tests of the HF against fully self-consistent results for interfaces. We saw no evidence for the anomalously large HF error reported in Refs. [2,3]. Our interfacial results are listed in Table I. In particular, we found only a 1% HF error for the Al(100) surface energy, whose value agrees well with that of an independent calculation [8].

It would be valuable to provide a quantitative identification of the source of the anomaly, but this was not done in Refs. [2,3] or in the preceding Comment [9]. In Ref. [6] we speculated that their large HF error was due to their [2,3] combining the results of separate bulk and surface calculations. However, without knowing the details of their computations we have no way of really knowing where the problem lies.

In all of the more than 70 calculations (9 interfaces, 8 to 9 interfacial spacings) we performed [6], we obtained good agreement between HF and fully self-consistent results. We believe that our results are the most complete test of the HF as applied to interfaces and surfaces to date. In all cases, our computations were a straightforward application of a very well-tested, first-principles method [10]. In particular, we did not have to contract or renormalize [2] our atomic electron densities or take any other steps to improve the HF accuracy.

We close with a comment about Table I. It is interesting that the HF accuracy is nearly the same for molecules, bulk solids, and interfaces. The HF error is due to a lack of self-consistency. It is well known that self-consistency is more difficult to obtain in surfaces and interfaces than it is for bulk solids and molecules because of the propensity for “sloshing” in the former (i.e., electronic densities move back and forth through the unit cell during interactions to self-consistency). One might have expected therefore that the HF errors would be larger for interfaces than for bulk solids or molecules. Harris [1] appears to have avoided this potential problem by writing the “double counting”

terms in his functional [second and third terms on the right-hand side of Eq. (2) of Ref. [6]] in terms of the *input* rather than the *output* electron densities.

In conclusion, we have established that the HF errors reported by Finnis *et al.*, are anomalously large based on our more than 70 HF and fully self-consistent interfacial calculations and HF calculations by many others. Therefore, we stand by our original conclusion that HF errors of order 10% can be found for interfacial energy computations. Further definitive work is required to determine why Finnis *et al.* obtained such large errors.

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- [1] J. Harris, Phys. Rev. B **31**, 1770 (1985); W. Matthew, C. Foulkes, and R. Haydock, Phys. Rev. B **39**, 12520 (1989).
- [2] M. W. Finnis, J. Phys. Condens. Matter **2**, 331 (1990).
- [3] A. J. Read and R. J. Needs, J. Phys. Condens. Matter **1**, 7565 (1989).
- [4] N. Chetty, K. W. Jacobsen, and J. K. Norskov, J. Phys. Condens. Matter **3**, 5437 (1991).
- [5] H. M. Polatoglou and M. Methfessel, Phys. Rev. B **37**, 10403 (1988); **41**, 5898 (1990).
- [6] J. R. Smith, T. Hong, and D. J. Srolovitz, Phys. Rev. Lett. **72**, 4021 (1994).
- [7] O. F. Sankey and D. J. Niklewski, Phys. Rev. B **40**, 3979 (1989); G. B. Adams and O. F. Sankey, Phys. Rev. Lett. **67**, 867 (1991); A. Caro, D. A. Drabold, and O. F. Sankey, Phys. Rev. B **49**, 6647 (1994).
- [8] K.-P. Bohnen and K.-M. Ho, Surf. Sci. **207**, 105 (1988).
- [9] M. W. Finnis, R. J. Needs, and U. Schönberger, preceding Comment, Phys. Rev. Lett. **74**, 3083 (1995).
- [10] See, e.g., J. R. Smith, J. G. Gay, and F. J. Arlinghaus, Phys. Rev. B **21**, 2201 (1980); T. Hong, J. R. Smith, D. J. Srolovitz, J. G. Gay, and R. Richter, Phys. Rev. B **45**, 8775 (1992); J. R. Smith, J. Ferrante, P. Vinet, J. G. Gay, R. Richter, and J. H. Rose, in *Chemistry and Physics of Fracture*, edited by R. M. Latanision and R. H. Jones (Nijhoff, Boston, 1987); J. G. Gay, J. R. Smith, Roy Richter, F. J. Arlinghaus, and R. H. Wagoner, J. Vac. Sci. Technol. A **2**, 931 (1984); X. Zhu, J. Hermanson, F. J. Arlinghaus, J. G. Gay, R. Richter, and J. R. Smith, Phys. Rev. B **29**, 4426 (1984).

TABLE I. Average HF errors.

	Energy error (%)	Spacing error (Å)
Molecules ^a	10	0.05
Bulk ^b	10	0.06
Interfaces ^c	11	0.03

^aRef. [1].

^bRef. [3–5].

^cRef. [6]; see also Ref. [7].