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Dr. Larry Cooper
Office of Naval Research
800 North Quincy Street
Arlington, Virginia 22207

Dear Larry,

I want to send you a brief letter describing a couple of papers that have been accepted for publication, and a couple of abstracts of papers to be delivered soon.

The first concerns an application of non self-consistent methods, especially the Harris functional, to an alloy problem. The present paper addresses the alloy AlTi, but its main purpose was to show that with a little care, non self-consistent methods can work essentially as well as fully self-consistent ones. Perhaps I mentioned to you on the telephone that I've mostly completed another paper on the Harris functional—intended for submission to Physical Review Letters—that demonstrates this claim much more generally and forcefully.

The Harris approach is important for several reasons. Finding efficient approaches is key to tackling many of the current problems of contemporary interest in electronic structure. This is because many of them, such as surface and interface problems, defects etc., involve a large number of atoms. For the same reason, molecular dynamics simulations are now limited by the efficacy of the electronic structure algorithms needed to obtain the total energy and forces. However, fully self-consistent solutions are hard to come by in large systems–the larger the system, the slower convergence to self-consistency. Worse yet, each iteration is slow for large systems, the time increasing as the cube of the number of atoms considered in the usual approaches. This is why there are preciously few *ab initio* calculations of large systems. When the Harris functional works well enough that we can skip self-consistency, it will be possible to treat large systems much more efficiently. Just as importantly, it paves the way to other schemes that would be difficult, if not impossible, to implement if self-consistency were necessary. For example, an *ab initio* version of the recursion method of Roger Haydock, might now be implemented in the context density-functional theory, using a non self-consistent Harris functional. Real-space approaches scale only linearly with the number of atoms in the system (rather than the cube), and make a highly attractive alternative—provided that they can be implemented within the context of density-functional theory. The Harris functional can supply the essential link connecting density-functional theory to the recursion method. Similarly, still more approximate, but more efficient schemes, stand a better chance of being successful, since they can now be carefully tested by detailed comparison to the

Harris functional. In particular the Gordon-Kim functional replaces the Harris functional by making a local approximation to the kinetic energy as well as the potential energy. Should it prove to be adequate, it will make an extremely efficient scheme for total energy calculations: one that is well suited to molecular dynamics simulations.

I've enclosed another paper, presented at the last PCSI, that addresses the influence ionized dopants in the depletion region have on tunneling current in Schottky barriers. It showed that the ionized dopants in the depletion region actually disrupt the tunneling current only a little. This paper was interesting because the conclusions are counterintuitive—one might expect that the corrections to be large since point charges look a lot different from a jellium!

Also enclosed are some abstracts of papers that have been accepted for presentation. The first two, done with John Klepeis (formerly a student of Walt Harrison) will be be presented respectively at the June conference of the Northern California Chapter of the AVS, and at the national AVS meeting in October. The first paper traces the evolution of the Schottky barrier pinning position in (110) GaAs as fractions of a monolayer of atoms are deposited. The second examines the de-reconstruction of a free GaAs surface. The last three abstracts concern magnetic properties of Fe/Cr superlattices and TbFe alloys, done in collaboration with Frank Herman. While these are not of direct relevance to semiconductors, they proved to be a good testing ground for the LMTO programs.

We've also done some extensive work on local-density calculations of the pinning of Schottky barriers, which I'll send along shortly. We show that intrinsic (MIGS) fermi-level pinning is strong; but that the pinning level *does* depend on the metal overlayer, demonstrating that Tersoff's hypothesis—that the pinning position is a property solely of the semiconductor band structure—is incorrect. Also, we observed if defects are present *behind* the MIGS, they govern the pinning position, regardless of how strongly the MIGS pin. We did introduce an antisite defect into the calculation to explicitly demonstrate this point.

I've enclosed the report you requested on patents, publications, etc. It looks a bit silly for 1989, but 1990 should look better. SRI's business and contracts office will also send your counterpart the same report. I also preparing a new proposal as regards continuation of the project, to be sent within the next few days.

I hope this puts you better up to date as regards our activities and aims. Please accept my apologies for being lax in reporting results. I had held off, hoping to wait only until the more interesting results were complete. "Technical difficulties" slowed the output more than anticipated, with the result that I held off too long.

Sincerely,

Mark van Schilfgaarde

STATEMENT "A" per Dr. Larry Cooper
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1989 Publications Report for ONR contract N00014-89-K-0132.

A. Papers submitted to Refereed Journals: none

B. Papers Published in Refereed Journals: none

C. Books submitted to Refereed Journals: none

D. Books Published in Refereed Journals: none

E. Patents filed: none

F. Patents granted: none

G. Invited Presentations: none

H. Contributed Papers: none

I. Honors/Awards/Prizes: none

J. Graduate Students and Postdoctorals Supported: none