

Dedication



Otto F. Sankey

This volume honors Otto F. Sankey, Regents Professor of Physics at Arizona State University on the occasion of his sixtieth birthday. Otto has been a prime contributor to solid-state physics, biophysics and the methodology of simulation of materials.

Otto received a B.S. degree from the University of Missouri (St Louis) in 1973, and a Ph.D. in Theoretical Physics from Washington University (St Louis) in 1979, under the direction of Peter A. Fedders. After a postdoctoral stint at the University of Illinois at Urbana-Champaign, with John Dow in the theory of defects in semiconductors, he became Assistant Professor of Physics at ASU in 1983. Otto's research achievements are remarkably diverse, beginning with his Ph.D. work on the theory of atomic hopping, then moving into the theory of defects in semiconductors. In 1986, Otto and Roland Allen published a paper "Atomic forces from electronic energies via the Hellmann–Feynman

theorem, with application to semiconductor (110) surface relaxation". The paper was remarkable in its insistence that interatomic forces should be derived from the electronic structure, not from *ad hoc* empirical potentials, an idea that is now considered obvious, but a key departure in the eighties, and contemporaneous with the efforts of Car and Parrinello to achieve the same goal with plane wave pseudopotential methods and a "fictitious Lagrangian". By a sustained effort of several years, Otto and his students created the first edition of FIREBALL, a local orbital, *ab initio* density functional code to compute the electronic structure and dynamically simulate molecular, surface and bulk systems. The key paper, published with student Dave Niklewski in 1989 is now a classic of the area with more than 900 citations, and many innovations that have withstood the test of time, among them the confined pseudoatomic "fireball" orbitals. FIREBALL has strongly influenced the area of first principles simulation both directly as a tool, and as a guide to others for solving the self-consistent Kohn–Sham equations and extracting interatomic forces efficiently. Many papers in this volume highlight the successes of FIREBALL. Otto's work in the period included dozens of important studies on high-pressure phases of materials, some of the first studies of Bucky Balls, nanotubes, and clathrates, among a very great number of other topics. That crude but useful instantaneous measure of scientific impact, the "h-index", stands at an impressive 50 at this moment. According to ISI, Otto's work has been cited nearly 10,000 times.

Harbingers of a new interest for Otto's restless mind became apparent in the 90's with work on theoretical biophysics. With characteristic single mindedness,

he carried out one of the first *ab initio* calculations on DNA with then student James Lewis, formed collaborations with leading experimentalists, and has since contributed to a stunning array of problems in the area. His ability to get to the heart of the physics allowed him to get calculations of DNA electronic conductance that were in the right ball park when compared to experiment. This feat has helped to propel a whole new approach to DNA sequencing. He recently developed a remarkably efficient way of calculating the vibrational modes of particles as large as virus capsids while retaining the important atomic information.

We should note that Otto is still in his prime, and we look forward to the next Festschrift at 70! We dedicate this volume with respect and affection for Otto, and look forward to many more years of friendship and collaboration.

David Drabold
Alex Demkov
James P. Lewis
José Ortega
Wolfgang Windl
Stuart Lindsay



Participants in a recent workshop honoring Professor Otto F. Sankey held in Tempe, AZ, in January 2011