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This Week's Citation Classic

Cohen M L & Bergstresser T K. Band structures and pseudopotential form factors for fourteen semiconductors of the diamond and zinc-blende structures. *Phys. Rev.* **141**:789-96, 1966. [Dept. Physics, Univ. California, Berkeley, CA]

Accurate calculations of band structures and crystal potentials for electrons in 14 common semiconductors were presented. For some compounds these were the first band structures to be computed. Experimental data, especially optical and photoemission measurements, were interpreted using the theoretical results and predictions of optical structure were made. [The *SCI*® indicates that this paper has been cited over 595 times since 1966.]

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"I was happy to learn that our 1966 paper has been chosen to be a 'Citation Classic' The research described in the paper was a continuation of work I had done at Bell Laboratories (1963-64) which itself was an outgrowth of an earlier (1962) collaboration at the University of Chicago with James C. Phillips and David Brust.[1,2]

"In September 1964, I arrived in Berkeley (along with student unrest) as a beginning assistant professor of physics. Tom Bergstresser was a graduate student who had some previous experience in solid state theory research. I encouraged him to work with me and suggested that we attempt to accurately calculate the electronic structure of 14 well-known semiconductors. This suggestion was a bold one because straightforward, first-principles techniques were unable to yield accurate calculations for any semiconductors. Uncertainties of the order of electron volts were common, whereas our goal was accuracy in the range of a few tenths of an electron volt for all the semiconductors.

"My optimism was based on the earlier success I had and faith in the power of the new methods we were using. The approach was not a first-principles one, but rather a pseudopotential technique where three experimentally determined parameters were used to fix the crystal potential for each element. Hence, our task was to assemble the available data, interpret the measured spectra, extract the most reliable components, and use these to fix the potentials. The electronic band structure calculations were then done using computers. The results were continually monitored by checking against the measurements. Here Tom Bergstresser's critical abilities were invaluable. Soon patterns emerged and the potentials for the various elements became internally consistent. The multitude of experimental data for various materials, which originally appeared chaotic, lined up in an orderly fashion allowing us to make predictions based on the patterns alone.

"It is gratifying that our work has had impact on both experimental and theoretical research. On the experimental side, our results indicated how the data should be interpreted and organized. Many predictions were made which the experimentalists could try to 'shoot down.' In subsequent years, we won most battles and surprisingly, even in the last few years, some experimental assignments of energy levels have been changed (because of better data) to be consistent with our 1966 results.

"The influence of our work on theoretical research which followed developed along several lines. Our approach, which is now usually called the Empirical Pseudopotential Method or the EPM, was applied to dozens of crystals, refined, amplified, and analyzed in detail.[3] The potentials which we fit with only an eye to semiconductor compounds were extracted and used for many other problems on metals, insulators, semiconductors, and semimetals. The energy level assignments stimulated general theoretical research on the origins and structure of optical spectra, crystal bonding, and electron interactions.

"I think the reason this paper receives many citations is partially because of the tremendous growth of research in this field. Also, one can obtain information about a relatively large number of popular semiconductors in one single source. Even though some of the work on individual semiconductors has been superseded, the basic results given in the paper are still reasonably accurate by current standards."

1. **Cohen M L & Phillips J C.** Spectral analysis of photoemissive yields in Si, Ge, GaAs, GaSb, InAs and InSb. *Phys. Rev.* **139**:A912-20, 1965.
2. **Brust D, Cohen M L & Phillips J C.** Reflectance and photoemission from Si. *Phys. Rev. Lett.* **9**:389-92, 1962.
3. **Cohen M L & Heine V.** The fitting of pseudopotentials to experimental data and their subsequent application. *Solid State Phys.* **24**:37-248, 1970.