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This Week's Citation Classic

Animalu A O E & Heine V. The screened model potential for 25 elements.
Phil. Mag. **12**:1249-70, 1965.
[Cavendish Laboratory, Cambridge, England]

Starting from the information available in the atomic energy spectra of the elements, the paper presents tables of the Fourier transforms of the effective self-consistent potential energy function, called pseudopotential or model potential, for the motion of valence electrons in solid or liquid states of the elements for various applications. [The *SCI*® indicates that this paper has been cited in over 670 publications since 1965.]

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"The inventions of the transistor and the solar cell for the space programme in the 1950s were major technological achievements resulting from solid-state physics research in the pre-World War II and immediate postwar periods. Further theoretical research into the electronic structure of metals and semiconductors received a new impetus when the concept of pseudopotential was introduced by James Phillips and Leonard Kleinman[1] at Chicago in 1959. The pseudopotential represents the effective self-consistent potential energy function that determines the motion of the conduction or valence electron in a material.

"At the Cavendish Laboratory, Cambridge, England, a sizeable experimental group had grown around the determination of electronic structure by various techniques; a complementary theoretical group was being assembled by John Ziman and Volker Heine around 1960. It was therefore exciting to work at the Cavendish Laboratory at that time.

"I arrived from Nigeria in October 1962 with a BSc degree in mathematics to do doctorate research under the supervision of Heine. Also at Cambridge that year was, among others, Igor Abarenkov, a visiting scientist from the USSR who, in order to avoid the complexity of the Hartree-Fock method of atomic structure calculation being used at the time, had originated the idea of solving the inverse problem, namely, to use the atomic energy spectrum to determine a 'model potential' for the motion of the electron. Volker immediately extended this idea to solids and showed that it worked quite well for aluminium (atomic number 13) and the alkali metals. Abarenkov left Cambridge in the spring of 1963, and Volker suggested the problem of extending the method to lead (Pb, atomic number 82) as my thesis project.

"Difficulties arose because the atomic energy spectral data for Pb were incomplete and a relativistic generalization of the method was required. To tackle both problems, I undertook, first, to predict the missing atomic energy data by studying the systematics of the atomic spectrum along rows and columns throughout the periodic table, and secondly, to devise methods of checking these predictions not only against the experimental data in solid and liquid Pb but also in all other elements in the periodic table for which data were available. In pursuit of this methodology, I visited many laboratories in the US in the summer of 1964 and in Italy in the spring of 1965. The reaction to my tables of the Fourier transforms of the model potential was very favourable, even among the pioneers in the field. At Cambridge there was not as much enthusiasm because of the risk factor in predicting the results for many elements where no experimental information was available, and for a while the results were distributed as preliminary. This produced a crisis situation in which I struck out on my own to issue these preliminary results as a preprint, in preparation for winding up my programme, if need be. As more favourable reactions reached Volker from the US with suggestions for improvement of the tables, we went back to work together and produced the final tables that were published in the *Philosophical Magazine* and in Walter Harrison's book.[2]

"Interest in the tables has persisted largely because they were readily accessible to experimental and theoretical solid-state physicists and the predictions turned out to be in agreement with subsequent data as detailed in a review article in 1970.[3] Further extension of the method to the transition metals took place between 1972 and 1976 at MIT's Lincoln Laboratory, where I also wrote a book[4] employing the pseudopotential method extensively."

1. **Phillips J C & Kleinman L.** New method for calculating wave functions in crystals and molecules. *Phys. Rev.* **116**:287-94, 1959.
2. **Harrison W A.** *Pseudopotentials in the theory of metals.* New York: Benjamin, 1966. 336 p.
3. **Cohen M L & Heine V.** The fitting of pseudopotentials to experimental data and their subsequent application. *Solid State Phys.—Adv. Res. Appl.* **24**:37-248, 1970.
4. **Animalu A O E.** *Intermediate quantum theory of crystalline solids.* Englewood Cliffs, NJ: Prentice-Hall, 1977. 516 p.