

Semiconductors: A pillar of pure and applied physics

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We give an overview of the central role semiconductor research that has played in basic, applied, and computational science. Our focus is on basic science. However, we will make general comments about applications, such as the transistor, integrated circuits, solar devices, and lasers, which evolved from basic research, and about simulations using computational science, which has enormously benefited from semiconductor research. We will make reference to links with other branches of physics and more generally other areas of science and fields like electrical engineering, computer science, material science, medical science, and chemistry that have made significant contributions to our everyday life. © 2015 AIP Publishing LLC.

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I. INTRODUCTION

Semiconductor studies influence many intellectual and conceptual aspects of physics. Studies of the electronic structure of semiconductors have influenced a large part of the theoretical foundation of modern condensed matter physics and materials science. Studies of correlation effects and interactions between elementary excitations (EE) in semiconductors led to the discoveries of the quantum Hall effects, fractional charges, new superconductors, topological insulators, and have influenced a number of other areas of research, which have become among the most active current topics in condensed matter physics. Some of these studies have influenced other parts of physics, chemistry, and engineering. Semiconductor research has been highly recognized. Starting with the transistor, ten Nobel Prizes in Physics have been awarded for research in this field.

After a brief discussion of some of the early history of studies in condensed matter physics, more recent developments will be described to illustrate the genesis of the modern models of a solid and the role that semiconductor studies have had.

II. EARLY HISTORY

It is likely that the earliest classifications of solids involved measuring mechanical properties like hardness. Scratch tests became the standard technique for hardness, and Mohs' scale developed in 1812 was a standard way to classify materials. Chemical composition is another classification scheme for materials, and the development of x-ray structural studies of crystalline solids allowed yet another convenient approach for classifying solids. However, materials with the same chemical composition can have very different properties, and crystals with the same structure but different atomic composition can also vary considerably. Probably the most important approach for classifying solids

is to measure their electrical resistivity and to group the materials according to the sizes of their resistivity.

The resistance of materials to the flow of electrical current varies significantly. In fact, static resistivity can vary over 35 orders of magnitude, and we are familiar in everyday life with these differences in materials like copper and quartz with resistivity of around $10^{-8} \Omega \text{ m}$ and $10^{17} \Omega \text{ m}$, respectively. The differences in materials are even more apparent if we look at the frequency dependence of the resistivity by measuring optical properties of solids. This will be discussed later, but when dealing with just the static or DC resistivity of solids, patterns emerge which are very useful for classifying materials. Table I lists the approximate resistivity values separating metals, semimetals, semiconductors, and insulators. Although these regions overlap and further distinctions are needed to clarify the boundaries, the general grouping is very useful. The grouping and refinements will be discussed later in terms of an electronic theory of solids.

The early history of theoretical studies of solids from a microscopic point of view depended on the acceptance of the atomic model of solids. Around 1900, the fact that matter was made of atoms was not universally accepted, and the theories of Boltzmann and Einstein for gases to explain phenomena, such as Brownian motion were just "taking hold." Einstein's thesis on measuring sugar molecules, his Nobel Prize winning paper¹ on the photoelectric effect, and his seminal paper² on the temperature dependent heat capacity of diamond helped to establish the atomic nature of solids

TABLE I. Resistivity categories of solids (in $\Omega \text{ m}$).

Category	Resistance	Example
Metal	10^{-8}	Copper
Semimetal	10^{-5}	Bismuth
Semiconductor	10^{-4} to 10^{+11}	Silicon
Insulator	10^{+16} to 10^{+24}	Diamond

and the beginning of quantum theory. Studies of the properties of gases, especially the optical properties of atoms and molecules helped establish quantum theory as it developed in the 1920's. By 1929, there was the challenge by Dirac³ that for this area of physics, quantum theory could explain all, but the solutions of the equations were difficult. Dirac and Fermi provided the statistical physics for Fermions that together with Boltzmann's theory for Bosons allowed many calculations of properties of solids. An excellent summary of these achievements is the 1933 review by Sommerfeld and Bethe.⁴ This marvelous review reads like a modern undergraduate book on solid state physics.

III. MORE RECENT HISTORY

Despite the advances made using quantum theory for a model calculation based on the properties of a box of free electrons with a jelly-like positive background to simulate the lattice, a detailed electronic structure calculation for a specific material, particularly semiconductors, remained generally unattainable until the 1960's. The latter advance relied heavily on the studies done on the optical properties of semiconductors. For the period 1940–1960, methods for calculating electronic structure of specific materials were being developed, but successes were not common. The dilemma of mathematically expressing a wave function for an electron in a solid was that for spatial regions near the nucleus the wave function is atomic-like, whereas between atoms, electrons behaved like they were free and plane wave states can be used. Hence, combinations of plane waves and localized atomic-like states appeared to be good basis sets. Slater⁵ introduced the Augmented Plane Wave (APW) method which essentially provided a numerical scheme following this approach. Herring⁶ introduced the Orthogonalized Plane Wave (OPW) method, where the effect of making a plane wave orthogonal to all the core states was to make the resulting wave function resemble the next higher state above the core states. Variations on these two methods led to important advances and some useful calculations.

However, even as extremely important advances were being made in condensed matter physics, electronic structure calculations that accurately described specific materials were rare. Even in 1957 when the Bardeen, Cooper and Schrieffer (BCS) theory,⁷ of superconductivity was developed, an accurate knowledge of the electronic band structure $E(k)$ of silicon was not available as was pointed out by Herring. However, 14 band structures for semiconductors were available by 1965.⁸ These band structures were computed to a high accuracy using a semi-empirical approach called the Empirical Pseudopotential Method (EPM). This approach required experimental input to fix the atomic potentials. The result was not only accurate calculations of the band structures (electronic energy dependence on wavevector), $E(k)$'s, but an interpretation of the optical spectra for many semiconductors and insulators in the visible and ultraviolet was obtained. An international collaboration of experimentalists and theorists in the late 1960's to the late 1970's⁹ essentially solved the puzzle of interpreting the optical properties of dozens of semiconductors and insulators and gave a better

understanding of optical properties more generally. The wavefunctions obtained using the EPM provided a theoretical microscope to visualize electron densities in solids.¹⁰

In the 1980's extensions to more first-principles approaches enabled successful calculations of the structural properties of semiconductors. These in turn led to explanations and predictions of superconducting, surface, interface, and high-pressure properties. By the 1990s', calculations for more complex materials and nanostructures became possible, and today, calculations of this kind are commonplace, and computer codes are available for non-specialists to do a large variety of calculations.

Whereas the view of many in the 1960's concerning computer-aided theory was not positive, it is rare to find theorists today who do not appreciate the power of this tool for modeling and simulation. What may not be fully appreciated is the fact that in the process of doing simulations, researchers discovered what were the most important contributions to the physical terms in a calculation. After revelations of this kind, it was possible to understand, physically and mathematically, why the numerical results signaled what one must focus on and what can be ignored.

This relationship between computational and scientific advances is a unique feature of semiconductor research, especially when one considers the role of material like silicon. Silicon is an extraordinarily important technological and computational material in constructing computer components; however, it is also an extraordinarily important "scientific material." Historically silicon has served as the notable benchmark for computational studies on semiconductors. Many theoretical "firsts" that have occurred using computers based on silicon to study silicon. For example, the first realistic band structures for semiconductors centered on understanding the electronic structure of silicon. The first analysis of optical, dielectric, and photoemission properties of solids involved comparisons to silicon. The first structural and high pressure studies of semiconductors used silicon as a testbed. The first "*ab initio*" molecular dynamics studies examined liquid silicon. Also, the role of quantum confinement at the nanoscale was first verified by calculations of the optical gap in silicon quantum dots. The importance of computer centered studies based on silicon computers is typified by the phrase "*in silico*," which is analogous in the way "*in vitro*" is used in biology.

Progress in semiconductor science is not only a result of more powerful computers; it is also a result of new algorithms and physical concepts. When the first computational studies were done with the EPM, computers were used to solve eigenvalues that involved a diagonalization problem that today could be solved on a cell phone. The number of atoms in the unit cell was typically less than a few dozen atoms at most. In the case of silicon, no more than a couple of atoms were involved. Today, the number of atoms can be more than 10000, or roughly three orders of magnitude larger.^{11,12} Typically, the electronic structure scales as the cube of the number atoms. If we use this scaling as a guide, the increase in the computational load would be 10^9 or more. Not all of this computing power comes from hardware. Moore's law would account for no more than 10^6 at best.

The key factor is that new algorithms have dramatically enhanced our ability to handle large scale problems. For example, new methods of diagonalizing large matrices based on iterative procedures typically run several orders of magnitude faster than those used in the 1960's.^{11,12} Another matter concerns the wave functions. While plane wave bases are easy to implement and are appropriate for crystals where translational symmetry exists, they have several limitations, especially for localized systems, such as molecules, clusters, and nanocrystals. Since plane wave bases are “infinite” in extent, they require global communications when implemented on parallel computers. This limits the scaling of the system size when the electronic structure problem is implemented on highly parallel systems. Moreover, a lack of periodicity necessitates the use of artificial symmetry to preserve translational symmetry when plane wave bases are used. Typically, super cells are used with plane waves. These cells are required to be large to isolate the localized system of interest and as such require large numbers plane waves. These issues can be overcome with real space methods wherein the electronic structure problem is solved using high order finite difference methods.^{11,12} These methods currently hold the “record” for the number of atoms that can be described by electronic structure methods.

IV. MODEL OF A SOLID: STRONGLY INTERACTING ATOMS

How do we explain and predict properties of solids now that we have the lessons taught to us by quantum theory, experimental investigations, and computer modeling? We know that quantum theory is appropriate and sufficient and that solids are made of atoms and atoms are made of nuclei, core electrons, and valence electrons. We also know that the predominant interactions are electromagnetic since gravity is too weak, and the weak and strong forces are too short-ranged. However the fact that there are of order 10^{23} particles/cm³ complicates matters significantly and allows effects, such as screening of the electromagnetic interactions. Hence, the latter have to be treated as non-instantaneously in addition to position dependent. Many researchers have spent a major fraction of their careers on the problem of an interacting electron gas in a box with a featureless compensating positive charge background to represent a solid. Although a great deal has been learned from these studies to calculate properties of real materials, the crystal structure, and the nature of the atoms making up the solid must be included. In what follows, the current approaches to exploring materials will be described.

One *standard model* of a solid treats a solid system as composed of strongly interacting atoms. For the discussion here, we will also assume that for most problems of interest, such as bonding properties, the solid can be pictured as composed of pseudo-atoms where the nuclei and core electrons are treated as a unit, i.e., positive cores. The valence electrons are pictured as being more or less itinerant and free to participate in bonding and other properties. As an example, for silicon, a pseudo-atom core contains a nucleus and 10 inert core electrons that together yield a net positive core

charge of +4. The cores are arranged in a four-fold coordinated diamond lattice, and the valence electrons move through the array of cores interacting with each other and with the cores.

A central question is the determination of the potential produced by the cores for the valence electrons. Since we are dealing only with the valence electrons, the potential needed involves both the nuclei and the core electrons, and this is called the pseudopotential. A major contribution of the core electrons in addition to screening the nuclear potential is to produce a repulsive potential arising from the Pauli Principle that restricts the valence electrons from occupying core states. A typical form of the potential is shown in Fig. 1. A Fourier transform of the potential for a given structure allows the determination of the energy band structure, $E(k)$, usually knowing only a few Fourier coefficients of the potential for each type of atom making up the solid. The number of coefficients needed depends on the crystal structure. For Si and Ge calculations, only three parameters (form factors determined from the Fourier coefficients) and the structural parameters, such as the lattice constant, are needed to give an accurate band structure (e.g., Ge in Fig. 2) over a range of order 20 eV.

The EPM form factors were obtained from experiment using primarily optical data. Manuel Cardona was a pioneer in measuring optical data and interpreting them. His early work involved reflectivity measurements, and after modulation spectroscopy was developed, he and members of his group studied many semiconductors and interpreted the spectra in terms of interband transitions.⁹ A major strength of this work was the comparison of optical structure for different materials that led to a classification of great use to theorists. Cardona also did seminal work on the pressure and temperature dependence of optical transitions that further classified their nature.

On the theoretical side, the EPM was capable of producing band structures, densities of states, optical spectra from calculations of the frequency dependent dielectric function, and even successfully predicted electron densities as shown

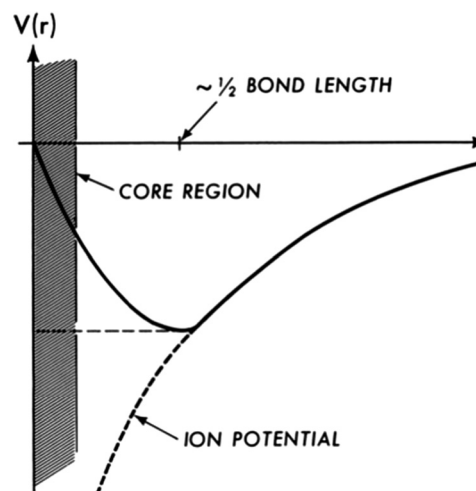


FIG. 1. Schematic pseudopotential in real space. The core region contains chemically inert states, which are not bound by the pseudopotential.

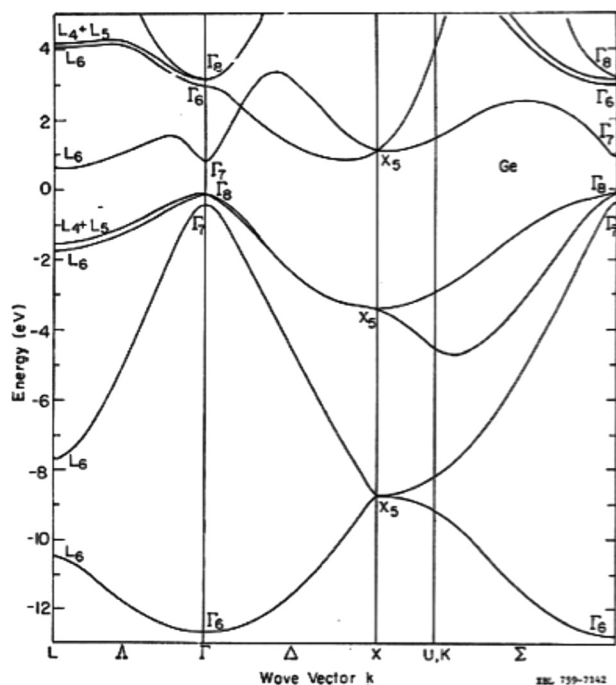


FIG. 2. Energy band structure for germanium. The top of the valence band is taken to be the energy zero.

for Si in Fig. 3. The density plot showed that in addition to producing energy levels correctly over a wide region, the associated wave functions were also reliable outside the core regions. Many conceptual problems concerning the properties of the electronic interactions were posed and solved using EPM studies. For example, it was shown that the EPM potential obtained for semimetals and metals “extracted”

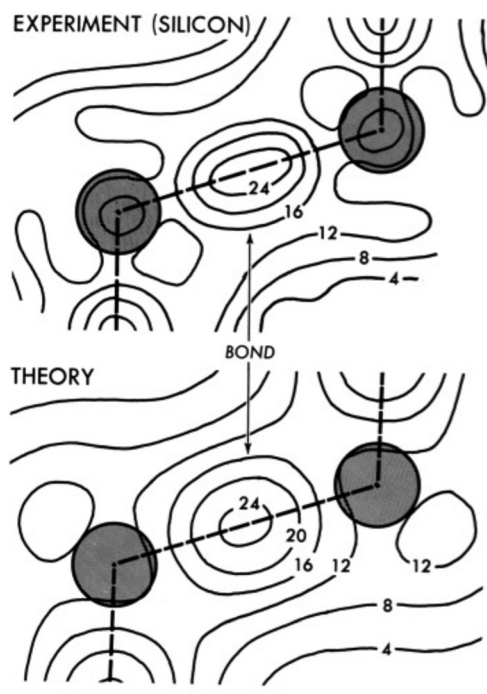


FIG. 3. Charge density map for silicon. Experiment is from Y. W. Yang and P. Coppens, Solid State Commun. **15**, 1555 (1974).³⁵ Reproduced with permission from J. R. Chelikowsky and M. L. Cohen, Phys. Rev. Lett. **33**, 1339 (1974). Copyright 1974 American Physical Society.

from studies of compound semiconductors could be used to calculate their Fermi surfaces. So for the most part, these potentials were transferrable and could work in many different environments. As a result, the EPM laid the foundation for the so-called *Ab Initio* Pseudopotential Method (APM).

The APM is usually based on constructing a pseudopotential to produce an electronic wave function for an atom with the constraint that the wave function reproduces the all electron (valence) wave function outside of a certain radius and then decay smoothly into the core region (see Fig. 4). The basic idea is similar to the one introduced by Fermi¹³ in 1934 for alkali atoms. Hellmann¹⁴ introduced similar approaches, which were based on density functional theory (DFT) from Fermi. Potentials of this kind^{15–17} were used for calculating total energies $E(\text{total})$ for a given crystal structure by summing the contributions coming from interactions between the ion cores, $E(c-c)$, between the electrons and cores, $E(e-c)$, the electron kinetic of the electrons, $KE(e)$, and the Coulomb and exchange correlation energy for the electron-electron interactions, $E(\text{Coulomb})$ and $E(\text{exc-correl})$, respectively,

$$E(\text{total}) = E(c-c) + E(e-c) + KE(e) + E(\text{Coulomb}) + E(\text{exc-correl}). \quad (1)$$

Using the method described above, the $c-c$ contribution can be obtained using Madelung sums, the pseudopotential provides the $e-c$ contribution, and the electron density can be used to compute the remaining terms, including exchange and correlation via DFT.¹⁸ The technical scheme was developed^{19,20} and provided structural information about solids. For example, in the case of Si, computing $E(\text{total})$ for different structures²¹ allows a comparison of these energies at various volumes. Assuming that the lowest energy structure will be the observed structure at a specific volume (obtained through high pressure techniques), one can predict new structures of Si. In addition, this method could be used to calculate the transition pressure required to produce a structural phase transition. For a given structure, the dependence of the energy on changes in volume provided a measure of the bulk modulus of the structural phase, and the volume for

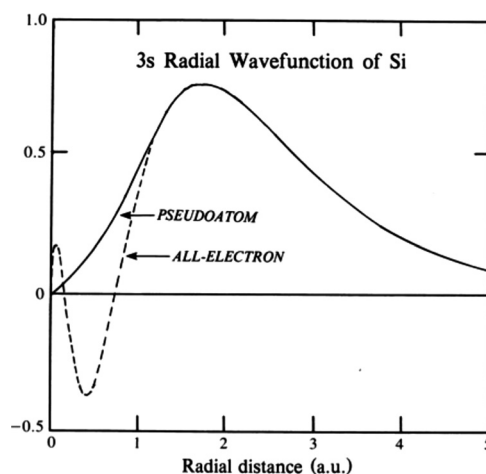


FIG. 4. All electron wave function (dashed line) and pseudopotential wave function (solid line) for the 3s state of the silicon atom.

which the energy of a phase is lowest gave a measure of the lattice constant. The results for these estimates are within around 1% for Si, and generally this is the accuracy found for most calculations of this kind. When one considers that only the structure and the atomic number are used as inputs, these results are impressive. In addition, many of the predicted high-pressure structures were found.

Another important results of this work were studies of the properties of vibrating lattices. By adding the input of the atomic mass, the APM was used to calculate vibrational spectra.²² One example of a technique in this area is the frozen phonon approach where the distortions caused by a specific phonon are put into the structure and the change in energy is computed. In practice, this method and other approaches developed later provided accurate calculations of phonon dispersion curves, Gruenisen constants, electron-phonon couplings, and a variety of lattice related properties.

The APM together with the EPM initially focused on crystalline semiconductors, but the methods were extended to other solids, clusters, molecules, and nanostructures. The basis set used for the wave functions is usually plane waves so that the starting point is a constant electron density. There are no built in features of the constituent atoms in the wave function basis. The bonding features of the electronic density develop in response to the atomic pseudopotentials in the course of a calculation. The APM and similar methods based on the interacting atoms model of a solid are considered a standard model for calculations in condensed matter physics (see Table II).

In addition to using the EPM and APM to calculate ground states and excited states²³ of semiconductors to explain their physical properties, these approaches were used for applications to explain properties of devices and to suggest paths for applications of semiconductors and other materials and also nano-material systems. We will discuss a few examples here. For semiconductor devices, often it is desirable to tailor a band gap for a specific application through alloying or structural changes. A rapid way to find applicable systems is to use methods like the EPM or APM to search for useful physical properties. This is often called “band gap engineering.” The methods can be applied to a broader range of devices, such as Schottky barriers or heterojunctions. These applications have, in some cases, led to new interpretations of the physics governing these devices through studies of electronic surface and interface states.

TABLE II. Partial list of properties that can be computed by the pseudopotential method.

Properties
Electronic structure (energy bands)
Crystal structures and phase stabilities
Hardness and mechanical stability
Vibrational and thermal properties
Electron-lattice interactions
Superconductivity properties
Optical and dielectric properties
Photoemission properties

Of particular recent interest in this general area is the tailoring of semiconductor properties to produce more efficient photoelectric devices. The most popular approach is the attempt to design materials with band gaps that can absorb solar radiation in the most effective way. This band gap engineering approach is one of the most popular. However, it is important to realize that obtaining a system with a band gap in the right energy range does not guarantee that a device built from this material will be efficient. It is more important to maximize the absorption coefficient in a desirable energy range to assure high absorption of the solar flux. An interesting study to illustrate this approach is to explore various structures of Si. In the diamond structure, the Si band gap is indirect, and the absorption coefficient is not very high for these transitions. Direct band gap semiconductors, such as GaAs where the top of the valence band state is p-like and mostly in the bond region while the conduction band state is concentrated near the As atom, have a p to s type transition in the gap region with a strong transition matrix element. The transition in Si is different. The valence band state is concentrated in the bond region, but the conduction band state is located in the interstitial region, and this results in a weak absorption. Hence, if modifications of Si are made where the basic bonding nature of the diamond structure is not changed, the transition is usually a weak one even if the modified Si is manipulated to be a direct band gap semiconductor. The situation can be drastically different if a different bonding configuration results by going to a new structural phase with an appropriate bonding configuration. Hence, it is important to use “wave function engineering”²⁴ in modifying semiconductors to maximize absorption in the desirable energy range. Fig. 5 illustrates this effect for diamond structured Si and Si in the R8 structure (referred to as modified Si in the figure). For the R8 case and some other structural phases of Si, a direct band gap can be obtained along with strong optical matrix elements.

Another important application of the APM relates to nanostructures, such as nanocrystals, nanowires, nanotubes, and nanofilms. An example of such calculations includes the description of how dopants behave in semiconductors at small length scales. Dopants, such as a P atom, have a Bohr radius of ~50 Å in crystalline silicon. If a nanocrystal of Si is much less than this size, one expects the dopant properties to be significantly altered. The physical properties of the dopant electron in small nano crystals are said to be altered by “quantum” confinement. Electronic structure methods can be used to describe this case, even though the host nanocrystal may include thousands of atoms.²⁵ In Fig. 6, the P dopant wave function is illustrated in a small nanocrystal of Si. In Fig. 7, properties of this P dopant electron are illustrated, including how the calculated hyperfine splitting energy of the electron compares to experiment. The general agreement between theory and experiment is a validation of the electronic structure description given by computation.

In most of the applications to bulk semiconductors, the bonding considered was sp^3 (as for the case of P in Si), and sometimes moderately ionic bonding, however for many nanosystems, the bonding nature is predominantly sp^2 . The three-fold coordination in graphene is a common example,

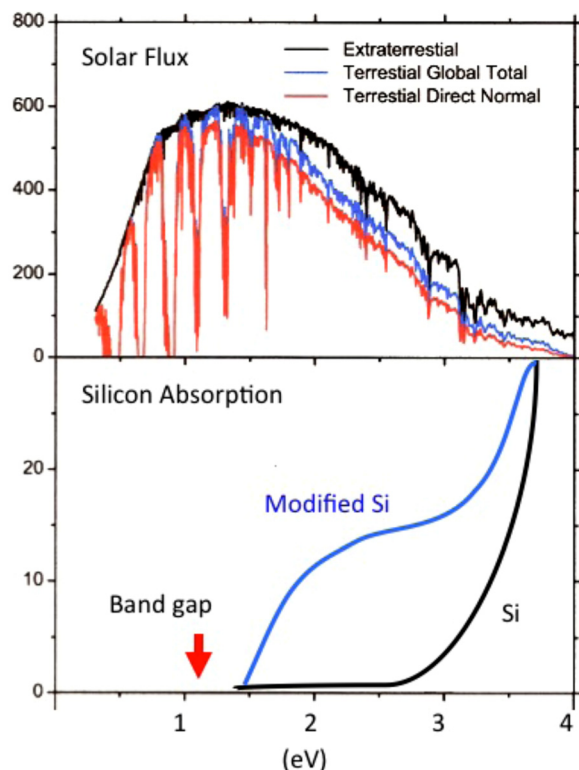


FIG. 5. Absorption spectrum (bottom panel) for crystalline silicon in the diamond and R8 structures, the latter labeled “modified silicon.” Also shown is the solar flux spectrum (top panel) using several standard measures.

and extensive research on properties of this material, and related systems, has been done. Here, we choose two examples related to nanotubes to illustrate the predictive power of the APM. Carbon nanotubes can be metallic or semiconducting depending on their chirality. Using electronic calculations and geometrical arguments, it is possible to design a Schottky barrier composed of a semiconducting carbon nanotube with lattice indices (8,0) and a metallic nanotube with indices (7,1) and join them with a 5/7 ring (see Fig. 8).²⁶ It can be shown theoretically that this system has

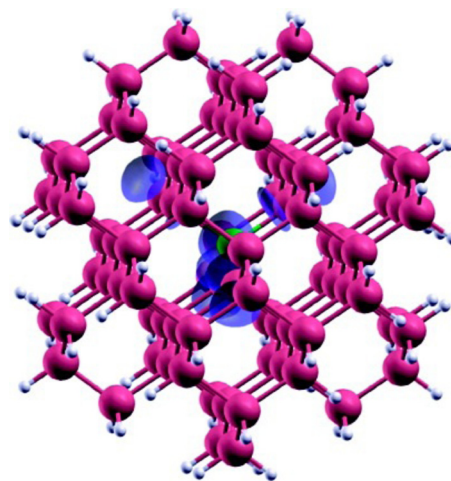


FIG. 6. Isocharge surface plot of the P donor electron state in a host Si nanocrystal. The Si atoms at the surface are capped with hydrogen like atoms.

properties similar to those of standard bulk semiconductor/metal junctions, but on a much smaller scale. These predictions were verified experimentally.

Another successful prediction^{27,28} was the boron nitride nanotube (BNNT) (see Fig. 9). In addition to showing that the BNNT should be stable, the electronic properties and the calculated tunability of the band gap with an electric field were shown to be correct. The use of BNNTs for various applications is growing because of the fact that these are wide band gap semiconductors for all chiralities with unusual properties when doped, such as a concentration of charge in the center of the tube when n-type. In addition, BNNTs serve as the pods for C₆₀ peapods, and unlike carbon nanotubes, the BNNT interaction with the enclosed C₆₀ molecules is small.

V. MODEL OF A SOLID: ELEMENTARY EXCITATIONS

Conceptually, the strongly interacting atoms’ model of a solid is a more accessible idea than the view that one can

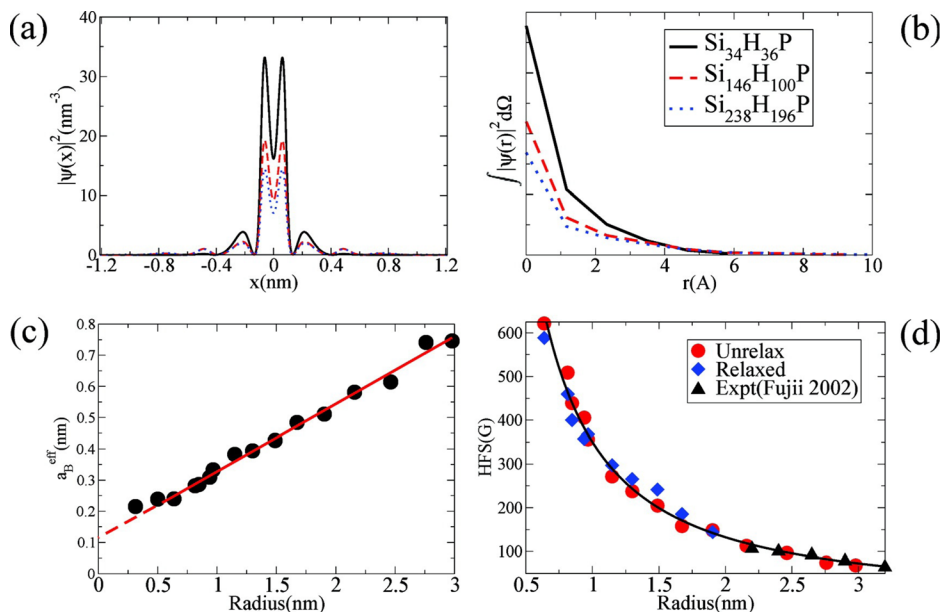


FIG. 7. (a) Charge density for the dopant electron along the [100] direction for three P-doped Si nanocrystals with different radii. x is the coordinate along that direction. (b) The corresponding spherically averaged charge densities. (c) The effective Bohr radius corresponding to the dopant electron as a function of nanocrystal radius. (d) Calculated hyperfine splitting of P-doped Si nanocrystals as a function of nanocrystal radius together with experimental data.²⁵ Theoretical values for both the unrelaxed bulk geometries and the fully relaxed structures are shown.

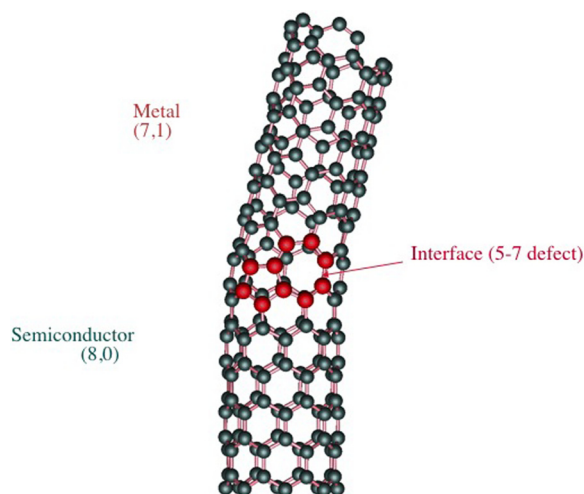


FIG. 8. (8,0)/(7,1) nanotube Schottky barrier showing an interface between a metal (7,1) and a semiconductor (8,0) tube structure. At the interface, a defect structure exists.

accurately describe the properties of a solid in terms of EE. Some of the concepts related to the EE model come from the ideas associated with emergence. In contrast to reductionism where it can be argued that if we are considering a solid made of atoms interacting via electromagnetic interactions, the rest is “turning the crank,” the EE approach states that properties or particles can emerge which can give a completely different view of what is happening and provide tools for exploring the nature of the system studied. It was mentioned earlier that the high densities of particles complicate the problem, but this feature can lead to interesting concepts. For example, the common notion of a hole in a semiconductor arose from the need to describe the absence of one electron in a gas containing of order 10^{23} cm^{-3} electrons. This positive “fictitious” particle adequately describes the system. It is viewed as a fermion quasiparticle with properties similar to an electron. A polaron is another particle in this class, whereas EEs associated with collective excitations, such as phonons, plasmons, and magnons are bosons representing vibrational, collective electronic, and magnetic waves,

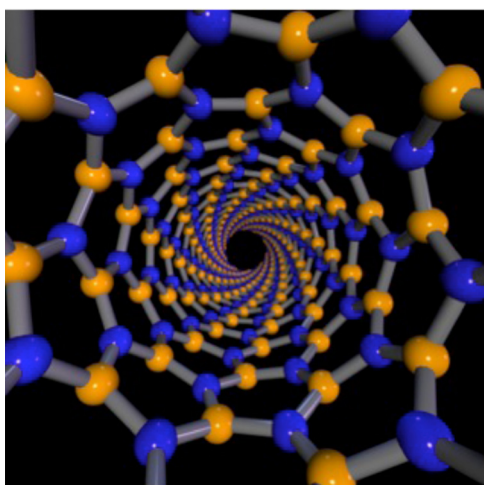


FIG. 9. A boron nitride nanotube.

respectively. This latter group’s properties are analogous to those associated with the wave/particle duality of light.

If we consider a solid as system with EEs composed of quasiparticles and collective excitations that “emerge” when the system is probed, then the task for the theorist is to calculate the response function that an experimentalist can measure. For example, for electromagnetic probes, the reflectivity can serve as the response function; for a temperature probe, it is the heat capacity; for a magnetic probe, it is the magnetic susceptibility. If a new state like ferromagnetism or superconductivity emerges, it should show up via probing and looking at a response function. It has been argued by Henri Bergson that “all we sense are images,” and thus in the model above, the description of the responses of a solid in terms of EEs is appropriate.

For semiconductors, the emergence of new robust states has proved to be an ideal venue where new EEs appear. The quantum Hall effect and the fractional quantum Hall effect where fractionally charged quasiparticles are detected are excellent examples. The existence of topological insulators with “protected” robust states is another. Magnetism and superconductivity have also been observed in semiconductor systems. Here, we choose to describe some research on superconductivity in modified semiconductors as an example of the use of the EPM and the APM to explore superconductivity of the conventional BCS type.

Since it is necessary to have mobile carriers to achieve a superconducting state, for semiconductor systems, doping and/or high pressures can be used to achieve this condition. Using knowledge of the early work of electronic band structure and doping properties,²⁹ it was possible to predict that a superconducting state could be achieved in doped semiconductors. This work led to the discovery of superconductivity in doped GeTe, SnTe, and SrTiO₃.^{30–32} A more relevant

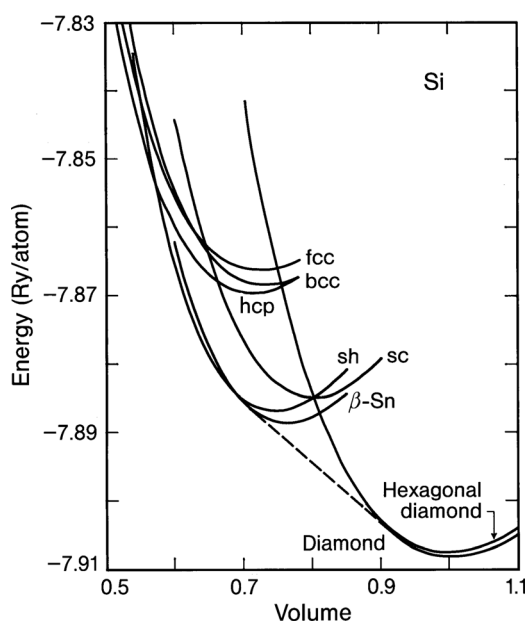


FIG. 10. Total-energy curves of the seven phases of Si as a function of the atomic volume normalized to the experimental volume. The dashed line is the common tangent of the energy curves for the diamond phase and the β -tin phase.³¹

study is the prediction of superconductivity in high-pressure phases of Si using the APM.³³

Two phases of Si were studied in detail, the simple hexagonal (sh) and the hexagonal close packed (hcp) structures.³⁴ Using energy/volume studies as described earlier (see Fig. 10), it was possible to predict successfully the existence of these phases and their stabilities, lattice constants, mechanical properties, electronic structure, phonon properties, electron-phonon couplings, and superconducting transition temperatures, including the pressure dependence of the latter. The theory was based on the BCS electron-phonon mechanism, and it has been suggested that Si may be the best understood superconductor since determining all of the above properties involved only inputs of the atomic number, atomic mass, the candidate structure, and the Coulomb μ^* potential obtained from the electron density.

VI. CONCLUSIONS

It is proposed here that semiconductor research has been a pillar of pure and applied science. Because of the vast and detailed experimental studies, semiconductors have been the focus of theoretical models and approaches. The models that were tested in detail for semiconductor systems became standard throughout condensed matter physics. It was found that a combination of approaches, such as the interacting atoms model and the elementary excitation model, gave excellent insight into the nature of solids in general. In addition, the techniques developed that were tested for explaining and predicting semiconductor properties became standard.

Because of the large number of applications of semiconductors and the many associated applied studies, this field demonstrated the need for cross fertilization between researchers working on basic and on applied science. There are many examples of mutual benefits.

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