

The Molecular Designing of Materials and Devices

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Abstract

Arthur von Hippel, a pioneer in the emergence of modern materials science, had a great goal: “the molecular designing of materials and devices.” In this article, I describe how computational materials theory has evolved over the last half century, helping to transform that goal from dream to reality. I start with two great puzzles of the 1950s: why band theory and the nearly free electron picture work. These were resolved by Landau’s quasiparticle theory and by pseudopotential theory, respectively. Together with the creation and development of density functional theory, key methodological advances, and the rapid evolution of computer hardware and software, these two insights have resulted in the achievement of the quantitative prediction of the structures and properties of complex materials. Bandgap engineering and design of multilayer multifunctional materials are given as examples of “molecular design.”

Keywords: *computational materials, electronic structure, molecular materials design.*

Introduction

Arthur von Hippel’s life and career spanned the entire 20th century, during which materials science emerged as a separate discipline having active interfaces with physics, chemistry, biology, and their applied and engineering correlates. In this issue of *MRS Bulletin*, we celebrate his many contributions to materials science and, in this article, I focus on one aspect of his prescient vision of how materials research can best be done.

Before World War II, von Hippel had already established his Laboratory for Insulation Research (LIR) at MIT, which, informed by his wartime experience in the power of interdisciplinary research, evolved into a prototypical materials research center. In the postwar LIR, a multidisciplinary effort involving both experiment and theory was brought to bear on Arthur von Hippel’s great goal, “the molecular designing of materials and devices.”¹

Here, I describe how materials theory—and in particular computational materials

theory—has evolved over the intervening years, helping to transform that goal from dream to reality (see Table I). It was a goal of the materials science field that I dreamed of myself, later than but independently of von Hippel.

I arrived at the University of Chicago in the fall of 1952, fresh from completing my PhD at the University of California, Berkeley, in solid-state theory under Charles Kittel. My position at Chicago was instructor in the Physics Department and the Institute for the Study of Metals (now the Franck Institute), another of the prototypical postwar interdisciplinary materials research centers. Soon after, I was called into the office of Cyril S. Smith, the founding director of the institute. He opened the discussion by asking (and I paraphrase), “What good are solid-state theorists?” Disconcerted, I stammered (and again I paraphrase), “We shall one day be able to design materials from first principles,” enunciating a theorist’s version of the great dream.

Smith was polite enough to display his skepticism nonverbally, and I did not predict when it might come to pass. It has come to pass now, half a century later, and is rapidly growing in reach and precision. In the following, I shall describe how it came about, starting with two of the great puzzles of the 1950s and their resolution, followed by a brief history of the emergence of the conceptual structure and methodologies that now make computational materials theory powerful enough for “the molecular designing of materials and devices.” Because of space limitations, I cannot systematically cover all the important developments in that vast field over so long a period. Instead, I have chosen to follow several threads through time, selected because they are representative and because of personal familiarity, not because I consider them necessarily more important or more central than those omitted.

Two Great Puzzles of the 1950s Why Does Band Theory Work?

The band theory, described in every textbook on solid-state theory, works! It provides a conceptual explanation of the distinguishing properties of metals, semiconductors, and insulators. Yet it is rooted in the independent-electron picture. Of course, it was also understood that electron–electron interactions were present and strong, comparable to all other energies. The many successes of band theory thus posed the deep question of how so many features of the independent-electron model survived in the presence of strong interactions. To add to the confusion, the Hartree–Fock approximation, the best one-electron approximation for the ground state, yields nonsense for the low-lying excited states of metals, a $-(T \ln T)$ dependence of the specific heat of metals on absolute temperature T at low temperatures.²

Why Does the Nearly Free Electron Theory of Metals Work?

It is tempting to dismiss the nearly free electron theory of metals of the elementary textbooks simply as a tentative step along the way to a “real” theory, and yet it works. As I stated in Reference 3:

The Hume–Rothery rules for the phase diagrams of noble metal alloys⁴ were explained by Jones⁵ on the basis of a nearly free electron model. Even more striking, the mean free paths of electrons in the alkali metals change only by a factor of two or so upon melting, remaining long above the melting point [despite the loss of the periodicity of the atomic structure of the crystalline

Table I: A Timeline for the Emergence of Computational Materials Science.

1955–2005	Evolution of computational power, algorithms, visualization tools
1956–1958	Fermi liquid theory
1959	Pseudopotential theory
1960–2005	Multiscale, hierarchical approaches
1964, 1965	Density functional theory
1973	Linearized basis sets
1973–1990	Further development of pseudopotential methods
1985	Car–Parinello method, quantum dynamics
1986	Quasiparticle spectra
1992–1996	Dynamical mean field theory

solid].⁶ Even for covalent insulators like diamond and silicon, the first band structure calculations for these materials yielded energy bands that were recognizable distortions of the free electron bands folded back into the first Brillouin zone.^{3,7–9}

More dramatically, Shoenberg and his students showed via the deHaas–van Alphen effect that the Fermi surfaces of the simple metals are weak distortions of the free electron sphere,¹⁰ as emphasized by Harrison.¹¹ For example, the relative deviation of the radii of the Fermi surfaces of Na and K from constancy is of order 10^{-3} – 10^{-4} .¹⁰ Again, it was understood that electron–atom interactions were present and strong, comparable to all other energies. The many quantitative successes of the nearly free electron theory thus posed the deep question of why those interactions failed to manifest themselves.

Key Conceptual Advances Fermi Liquid Theory

The first step toward a deep understanding of why band theory works was the introduction of Landau’s Fermi liquid theory of metals.¹² If adiabatic perturbation theory in the Coulomb interaction between electrons converges, there is a one-to-one correspondence between the eigenstates of an appropriate independent-particle system and a set of approximate eigenfunctions of the actual interacting-particle system. The low-lying states among the latter have finite but long lifetimes. The excitations of the independent-particle system, electrons above the Fermi surface and holes below it, stand in one-to-one correspondence to the excitations of the interacting system (quasiparticles), quasielectrons above and quasiholes below the Fermi surface of the metal. Ignoring phonons, the lifetime of a quasiparticle is inversely proportional to the square of its excitation energy and thus diverges at the Fermi surface. Although invented by Landau to explain

why the independent-electron model of metals appeared to work, the quasiparticle concept is even more powerful for semiconductors and insulators than for metals. There is a quasiparticle band structure. Ignoring phonons again and photons as well, a quasielectron in an empty conduction-band state can only lose energy by an Auger process in which a quasielectron is kicked up into the conduction band, leaving a quasihole behind in the valence band. The minimum energy required to create this quasielectron–hole pair is the bandgap. Thus, all quasielectrons excited into the conduction band by an energy less than the bandgap above the bottom of the conduction band have infinite lifetimes, and similarly for quasiholes in the valence band.

The formal theory of many-electron systems, which had been emerging since the 1930s, was given a sharper focus by Landau’s Fermi-liquid theory. For simple metals, the quasiparticle kinematics and dynamics turned out to differ little from those of noninteracting electrons. Nevertheless, exchange and correlation effects remained important. They play a major role in setting the value of the Fermi level. It is the dynamical screening of the exchange by electron correlation that restores the proportionality of the heat capacity to T . Electron correlation refers to the influence on the motion of each electron of the difference between its dynamical interaction with all others and its averaged interaction. The effects of electron–phonon interactions were sorted out, explaining the large effective masses of quasiparticles in the heavy simple metals. Two further early developments were of prime importance for many-body theory and for condensed-matter physics in general, the BCS (Bardeen–Cooper–Schrieffer) theory of superconductivity¹³ and the theory of the Kondo effect.¹⁴ As these and many later important developments have not been central to the emergence of first-principles computational materials theory, I shall not dwell upon them.

Pseudopotential Theory

The answer to why valence and conduction electrons behave as though they were nearly free in simple metals was provided by pseudopotential theory in the form introduced by Phillips and Kleinman¹⁵ within an independent-particle framework. They divided the electronic states into core states little affected by their presence in a material and valence/conduction states profoundly affected. For the latter, they introduced pseudowave functions, relaxing the requirement of orthogonality to the core functions. Instead, an additional repulsive potential was added to the Hamiltonian generating the pseudowave functions. Combined with the potential in the original Hamiltonian, it became known as the pseudopotential. The matrix elements of the pseudopotential important for determining the shape of the Fermi surface in simple metals and of the energy bands in simple semiconductors turn out to be small, whence their nearly free electron character. The repulsive potential is in fact a Pauli repulsion, arising from the requirement of orthogonality to the wave functions, and it is the kinetic energy introduced by the requirement of orthogonality that is captured by the repulsive potential and that cancels the attractive inner region of the atomic potential.¹⁶

The pseudopotential concept and its cancellation theorem¹⁶ have not only clarified the question of free-electron-like behavior, but have deepened our understanding of crystal structure^{11,17} and the properties of liquid metals,⁶ and clarified a broad range of chemical trends.

Density Functional Theory

The first goal faced in designing a material is the accurate determination of its stable ground-state electronic and atomic structures by minimizing the total energy of the system. While the conceptual advances provided by the quasiparticle and pseudopotential theories were fundamentally important, they did not advance us toward that goal. Pseudopotential and other preexisting or contemporary methods could accurately determine the states of a single electron in a given potential V , but the questions of how V should be determined and how the total energy would emerge from those states remained open. The Hartree approximation answered both questions too crudely. The Hartree–Fock approximation was both computationally intensive and gave poor results for certain properties of metals. Slater’s $X\alpha$ method simplified the Hartree–Fock equations by introducing a local approximation to the exchange

potential but incorporated an empirical parameter α .¹⁸

In 1964, Hohenberg and Kohn introduced density functional theory (DFT),¹⁹ showing that one could base the formal structure of many-electron quantum mechanics on the electron density in place of the many-electron wave function. This revolutionary insight was followed in 1965 by a demonstration by Kohn and Sham of the existence of an independent-particle system with the same ground-state electron density as the many-electron system.²⁰ Specific prescriptions were given for the potential V in which the electrons moved independently, and for the connection between total energy and the electron density, the density functional, answering the open questions posed earlier. Attention then focused on finding adequate approximations to the density functional and the Kohn–Sham potential V as well as on computational schemes to exploit the new insights.

Key Methodological Advances Linearized Basis Sets

Methods based on the pseudopotential concept proved computationally efficient for lighter atoms. M.L. Cohen and his students, in particular, thereby provided a quantitative theoretical basis for broad areas of semiconductor physics.²¹ In the 1960s, however, when pseudopotentials were first in wide use, they had limitations for application to oxygen, making oxides difficult, and for d and f states, putting transition metals, rare-earth metals, actinides, and their compounds out of reach. Schemes usable for such materials already existed, the augmented plane wave (APW) method of Slater²² and the KKR method of Koringa and Kohn and Rostoker.^{23,24} As formulated, however, they were too computationally intensive for the times. The problem was that the basis sets used in those methods were energy-dependent, so the matrix elements in the secular equation for the energies became energy-dependent, a major complication. In 1973, Anderson²⁵ showed that it was possible to linearize that energy dependence about a well-chosen energy without loss of accuracy, restoring the linear form of the secular equation. Such linearized methods were much less computationally intensive, and the entire periodic table became accessible.

Pseudopotential Methods: Further Developments

With pseudopotentials, a plane-wave basis can be used to expand the one-electron wave functions of the Kohn–Sham theory. Plane waves offer many

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advantages over more complex, atom-related basis functions. Quantities more efficiently computed in k -space such as the kinetic energy can be computed in the plane-wave basis set, but quantities more efficiently computed in real space can be computed there, with fast Fourier transforms allowing efficient passage between real space and k -space. Forces on nuclei are much easier to compute in a basis independent of nuclear positions. Consequently, systematic development of pseudopotential methods continued. These developments have been reviewed in Martin’s monograph on electronic structure.²⁶ The key developments were norm-conserving pseudopotentials,^{27,28} separable pseudopotentials,²⁹ and ultrasoft pseudopotentials.³⁰ The latter in principle opens the entire periodic table to electronic structure computations using plane-wave basis sets, subject to the limitations of the approximations used to construct the density functional, about which more later.

The Car–Parinello Method

Up through the mid-1980s, DFT was used to calculate the electronic ground-state energy for a preset nuclear configuration in the Born–Oppenheimer approximation. Varying the nuclear configuration then generated the potential energy surface on which the nuclei moved. Finally, one could minimize the nuclear potential energy to find the stable ground-state structure or use it in molecular dynamics. However, minimizing the electronic ground-state energy for each nuclear configuration is computationally very intensive.

In 1985, Car and Parinello³¹ found a way to accelerate the computation. In DFT via the Kohn–Sham theory, the total energy is a functional of both the set of occupied Kohn–Sham independent-electron spin orbitals and the set of nuclear coordinates. Car and Parinello pointed out that minimizing the energy for each nuclear configuration could be avoided by treating the Kohn–Sham spin orbitals as fictitious classical coordinates and introducing a classical dynamical equation of motion for them coupled to the classical

equations of motion of the nuclei. With damping terms judiciously added, it was found that computational efficiency was greatly enhanced in the search for ground-state electronic and atomic structures. Alternatively, the method could be run at finite temperature, generating an efficient quantum molecular dynamics. Pseudopotentials and plane-wave bases are particularly well adapted to this method, and therefore this method is in widespread use. Complex molecules, liquids, glasses, and many other systems have been studied.

Dynamical Mean-Field Theory

With these methodological advances, the accuracy of a calculation with a given density functional was no longer an issue. Instead, attention focused on two other limitations, the inadequacy of the existing approximations to the density functional for systems in which the electrons are strongly correlated and limitations on the size of the systems that can be tackled. I discuss progress with the first limitation in this section and with the second in the next.

Electron correlation becomes important when energy bands are narrow and electron–electron interactions are strong, both associated with relatively tightly bound valence and conduction electrons. Thus transition metals, rare-earth metals, and actinides and their compounds, with their more tightly bound d or f states, may contain strongly correlated electrons. The approximations to the density functional now in use for the study of materials have all evolved from the local density approximation, the so-called LDA,²⁰ which approximates the exchange and correlation energy density of a real system locally by that of a uniform electron gas of the same density. The electron density in strongly correlated materials varies rapidly, and nonlocal effects are important, so it is not surprising that the LDA and its improvements fail in these materials.

Bands are narrowest and interactions strongest among transition metals in the late $3d$ series. For example, while the total energy, lattice constant, and magnetic moment of ferromagnetic nickel can be satisfactorily calculated by standard DFT methods, these overestimate the Curie temperature by a factor of two. A somewhat ad hoc introduction of correlation fixes the error. Heavy fermion systems, valence fluctuations, and the complex phase diagrams of the actinides are beyond reach.

However, these have all been brought within reach by dynamical mean field theory (DMFT),³¹ which treats correlation effects explicitly in an approximation that

becomes exact when the coordination number diverges. DMFT computations require input information derived from standard DFT computations. There have been substantial recent successes.³² The computations are intensive, limiting the structural complexity of the materials studied, but it is still early in their history.

The Power of Evolution

We are all familiar with Moore's law; for five decades, computing power per unit cost has grown exponentially with time. Processing power doubles approximately every 18 months and memory capacity every two years. We are less familiar with its correlate relating to software instead of hardware. The codes we use for electronic and atomic structure computations have grown correspondingly in power. In the 18-year period between 1978 and 1996, there was a hundredfold increase in the size of treatable systems, a doubling every 2.7 years. At present, 1000 atom systems are accessible to a full quantum-mechanical treatment.

The factors involved in this dramatic growth are of course more powerful computers with more memory, better programming tools, bigger subroutine libraries, and commercially or publicly available evolving electronic-structure codes. Perhaps most important, however, has been the deepening of our understanding of the underlying theory and the recognition that with greater computing power and memory, more sophisticated and accurate theories can be implemented.

Another important factor is the emergence of powerful visualization programs, which enable us to make sense out of the flood of data emerging from the computations, thus taking advantage of the human brain's remarkable pattern-recognition ability.

There is no indication that this evolution of capability is slowing down.

Hierarchical Approaches

There are problems that, while feasible, are too complex to be treated directly with first-principles methods. The complexity can arise because the physical scale of the problem is too large. Examples are: (1) dislocation movement, which is atomic in scale at the core, but generates a time-dependent macroscopic strain field; (2) crack propagation, which is atomic in scale at the tip, with again a time-dependent macroscopic strain field; (3) grain growth, Ostwald ripening, and phase transitions, which are atomic in scale at interfaces but generate macroscopic changes in morphology; and (4) enzyme activity, which is atomic in scale at

the active site, but the overall catalytic mechanism involves much of the entire protein. Such problems could require simulations involving more than 10^6 atoms, which is not yet feasible if treated quantum mechanically. The strategy for dealing with this multiscale complexity is to use fully quantum mechanical methods at the atomic scale, couple these to classical molecular dynamics using model force fields at intermediate scales, and, if neces-

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sary, couple the latter to classical continuum methods for the fully macroscopic scale.

Alternatively, the complexity can be such that the number of atoms is not too large for simulation, but the number of iterations required to generate the information desired may be too large. In such cases, a successful strategy can be to map the fully quantum mechanical problem onto a much simpler dynamical or statistical mechanical model that is feasible to simulate. The parameters of the model are then generated by many fewer quantum computations. Examples are alloy bulk and surface phase diagrams for which the mapping is onto a generalized Ising model; ferroelectric films or multilayers, for which the mapping is onto a Landau-Ginzberg free energy functional, and trends in surface chemistry and heterogeneous catalysis, for which the mapping is onto a tight-binding model of electronic structure.

In the complex multiscale problems, the parameters of the force fields or the model Hamiltonian can be computed from relatively small quantum mechanical computations. The LDA computations on which the DMFT computations are built also provide such a mapping. Thus, there may be no clear boundary between the two strategies. One uses them when and where one needs them.

Finally, complexity can arise when one deals with electronic excitation processes in even quite simple systems, for example, in the optical absorption of semiconductors. Here the mapping can be onto a simplified Bethe-Salpeter equation with the quantities entering taken from LDA computations.³³ Alternatively, much effort is now going into the time-dependent generalization of DFT known as TDDFT; as the time-dependent density functional be-

comes better understood, one can expect substantial progress.

Concluding Remarks

But has all this progress resulted in "the molecular design of materials"? The answer is yes. The bandgap engineering of semiconductor device structures is now routine, with electronic structure computations as an essential component of the process.³⁴

I shall close with examples relevant to von Hippel's interests in materials of high dielectric constant and in ferroelectrics.^{1,35}

Polycrystalline $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ has an unusually high dielectric constant κ and is under consideration for high- κ applications. The κ of the single crystal reaches 10^5 . The central issue that had to be settled before applications might proceed was whether the high κ was intrinsic to the material or extrinsic. It was shown to be extrinsic by state-of-the-art first-principles computations of the electronic structure, phonon frequencies, Born effective charges, and the intrinsic value of the κ of the material.^{36,37} The latter turned out to be three orders of magnitude smaller than observed. Such computations on a material with 40 atoms per unit cell and an antiferromagnetic ground state were beyond imagining in von Hippel's time, yet the outcomes are very important to the materials he studied and have since become important for many commercial applications.

Finally, there are now research programs to design, via computations, and fabricate, via multilayer deposition techniques, complex multifunctional materials: multiferroics, ferroelectrics with interfacial-strain-enhanced properties, and other novel materials.

References

1. This is an allusion to *The Molecular Designing of Materials and Devices*, edited by A.R. von Hippel (MIT Press, Cambridge, Mass., 1965).
2. J. Bardeen, *Phys. Rev.* **50** (1936) p. 1098.
3. M.H. Cohen, *Physica B* **296** (2001) p. 7.
4. W. Hume-Rothery, *The Structure of Metals and Alloys* (Institute of Metals, London, 1936).
5. H. Jones, *Proc. Phys. Soc.* **49** (1937) p. 243.
6. T.E. Faber, *Introduction to the Theory of Liquid Metals* (Cambridge University Press, Cambridge, UK, 1972).
7. F. Herman, *Phys. Rev.* **88** (1952) p. 1210.
8. T. Woodruff, *Phys. Rev.* **98** (1955) p. 1741.
9. T. Woodruff, *Phys. Rev.* **103** (1956) p. 1159.
10. D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge University Press, Cambridge, UK, 1984).
11. W.A. Harrison, *Pseudopotentials in the Theory of Metals* (W.A. Benjamin, New York, 1966).
12. L. Landau, *J. Exp. Theor. Phys.* (USSR) **30** (1956) p. 1058; L. Landau, *J. Exp. Theor. Phys.* (USSR) **32** (1957) p. 59; L. Landau, *J. Exp. Theor. Phys.* (USSR) **35** (1958) p. 97.

13. J. Bardeen, L.N. Cooper, and J.R. Schrieffer, *Phys. Rev.* **106** (1957) p. 162; J. Bardeen, L.N. Cooper, and J.R. Schrieffer, *Phys. Rev.* **108** (1957) p. 1175.
14. J. Kondo, *Prog. Theor. Phys.* **116** (1964) p. 37.
15. J.C. Phillips and L. Kleinman, *Phys. Rev.* **116** (1959) pp. 287, 880.
16. M.H. Cohen and V. Heine, *Phys. Rev.* **122** (1961) p. 1821.
17. M.L. Cohen and V. Heine, in *Solid State Physics*, Vol. 24, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1970) p. 37.
18. J.C. Slater, *Phys. Rev.* **81** (1951) p. 385; *Adv. Quantum Chem.* **6** (1972) p. 1.
19. P. Hohenberg and W. Kohn, *Phys. Rev.* **136B** (1964) p. 864.
20. W. Kohn and L.J. Sham, *Phys. Rev.* **140A** (1965) p. 1133.
21. M.L. Cohen and J.R. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors*, 2nd ed. (Springer-Verlag, Berlin, 1988).
22. J.C. Slater, *Phys. Rev.* **51** (1937) p. 846.
23. J. Korringa, *Physica* **13** (1947) p. 392.
24. W. Kohn and N. Rostoker, *Phys. Rev.* **94** (1954) p. 1411.
25. O.K. Anderson, *Phys. Rev. B* **12** (1975) p. 3060.
26. R.M. Martin, *Electronic Structure: Basic Theory and Practical Methods* (Cambridge University Press, Cambridge, UK, 2004).
27. W.C. Topp and J.J. Hopfield, *Phys. Rev. B* **7** (1973) p. 1295.
28. D.R. Hamann, M. Schlüter, and C. Chiang, *Phys. Rev. Lett.* **43** (1979) p. 1494.
29. L. Kleinman and D.L. Bylander, *Phys. Rev. Lett.* **48** (1982) p. 1425.
30. D. Vanderbilt, *Phys. Rev. B* **41** (1990) p. 7892.
31. R. Car and M. Parinello, *Phys. Rev. Lett.* **55** (1985) p. 2471.
32. G. Kotliar and D. Vollhardt, *Physics Today* **57** (2004) p. 53.
33. M.S. Hybertson and S.G. Louie, *Phys. Rev. B* **34** (1986) p. 2920.
34. M. Peress, N. Binggelli, and A. Baldereschi, *J. Phys. D: Appl. Phys.* **31** (1998) p. 1273.
35. A. von Hippel, *Rev. Mod. Phys.* **22** (1950) p. 221.
36. L. He, J.B. Neaton, M.H. Cohen, D. Vanderbilt, and C.C. Homes, *Phys. Rev. B* **65** 214112 (2002).
37. M.H. Cohen, J.B. Neaton, L. He, and D. Vanderbilt, *J. Appl. Phys.* **94** (2003) p. 3299. □

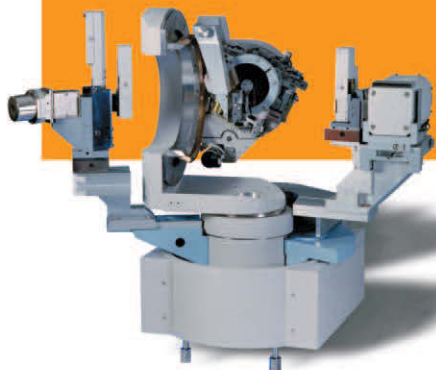


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