

ELECTRONIC STRUCTURE CALCULATIONS FOR MAGNETICALLY ORDERED SYSTEMS

Although magnetism was known to the ancients, its uses before modern times were very limited. The compass was probably the most important application before the 19th century. After Oersted's discovery, in 1820, that magnets interact with electric currents, the number of applications grew rapidly. The classical union of electricity and magnetism culminated, of course, in Maxwell's beautiful theory of the electromagnetic field.

The discovery of the electron's intrinsic spin, early in this century, showed us a new kind of magnetic source, not explicitly related to the motion of electric charge. After that it became possible, in principle at least, to predict the macroscopic magnetic behavior of arbitrary systems.

Maxwell's equations only provide us with a macroscopic theory. Properties of materials are parameterized via susceptibilities. But a proper microscopic theory requires the quantum theory of atoms, molecules and solids. The connection between microscopic and macroscopic descriptions is made as follows: Quantum electrodynamics couples the free-space electromagnetic fields to the quantum mechanical fields that describe matter. That's all one needs, in principle, for the description of magnetic phenomena.¹

For macroscopic systems it is, of course, much easier to separate external (macroscopic) from internal (microscopic) fields and solve the standard Maxwell equations on a macroscopic level, simply parameterizing the microscopic behavior of materials in terms of magnetic susceptibility. One does need quantum effects to evaluate susceptibility, but fortunately ordinary nonrelativistic quantum mechanics suffices.

The theoretical methods described in this article are valid for systems containing many atoms as well as for single atoms. Nowadays one can do calculations for a hundred atoms in a unit cell. The article on page 43, by David Awschalom and

Density functional theory calculated on fast computers is a powerful tool for describing magnetic phenomena in solids. It can even handle magnetic anisotropy in layered systems.

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David DiVincenzo, describes the fabrication of small magnetic elements with about that many atoms. In that sense experiment and theory are converging on a common ground.

Magnetic moments of atoms

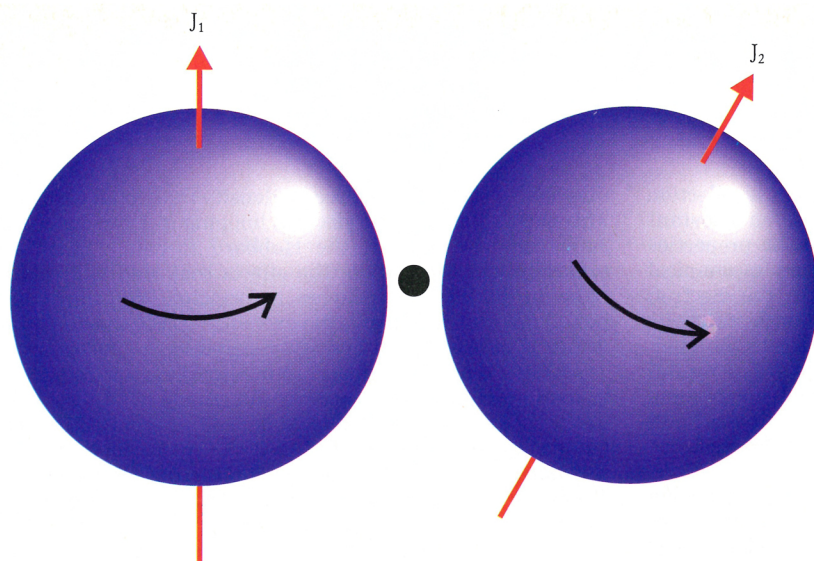
All magnetic properties of a solid are attributable to its electrons. In a free atom or ion, there are two contributions to the magnetic moment: First of all, every electron has intrinsic spin s and its associated magnetic moment. Then there is the magnetic moment associated with the electron's orbital

angular momentum l . In a free atom these contributions are typically comparable in magnitude. For all but the heaviest atoms we can use Hund's rules (see the box on page 51.) to predict the ground-state configuration of the electrons. Hund's rules assume that angular momentum states are well described by LS (Russell-Saunders) coupling. But that is a poor approximation for the heaviest atoms (the actinides), where jj coupling prevails. Our discussion here, which assumes the validity of Hund's rules, will therefore not be valid for the actinides.

To build up a net spin moment S , the individual electron spins have to point in the same direction. This alignment is due mainly to the Pauli principle. Because of the antisymmetry of the wavefunction under exchange, the probability of finding two electrons with the same spin orientation must vanish as they approach each other. Therefore electrons with parallel spins tend to be further apart than electrons with antiparallel spins, for which there are no Pauli-principle restrictions. Coulomb repulsion also favors configurations with larger distances between electrons. Thus one can say that the Pauli principle causes spin alignment. But the fact that Coulomb repulsion operates irrespective of spin orientation reduces the energy difference between parallel and antiparallel pairs and hence lowers the degree of spin alignment.

The formation of mag-

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HEISENBERG EXCHANGE interaction energy between two localized magnetic moments with angular momenta $\mathbf{J}_1$ and $\mathbf{J}_2$ is proportional to $\mathbf{J}_1 \cdot \mathbf{J}_2$. The sign and magnitude of the proportionality constant depend on details of the electron configurations. **FIGURE 1**

netic moment in atoms has been studied in great detail.² Nowadays one can perform full quantum mechanical calculations for light atoms to obtain their electronic configurations without resorting to simplifying approximations. One finds that the individual contributions of spins and orbits to the total magnetic moment follow Hund's rules quite nicely. One can't do these complete calculations for heavier atoms, because the complexity of the quantum mechanical problem scales exponentially with the number of electrons. We do, however, have very good approximate results for heavier atoms, and the formation of atomic magnetic moments is well understood.

Magnetism in solids

The situation is quite different for solids. There the number of electrons involved is extremely large, and complete calculations are never possible. It is therefore very useful to have simple models that describe magnetism in solids to first approximation. These models give us the vocabulary needed to discuss magnetism in real, complicated systems like magnetoelectronic devices.

One way of describing the formation of a solid is to think of individual atoms being brought together, each carrying its own magnetic moment. Because atomic moments are localized, such models describe localized magnetism in the solid. But because the atoms are not infinitely far apart, electrons can hop from atom to atom. In this way they carry information about the magnetic state of one atom to another. In models of localized magnetism this hopping does not occur rapidly. Most of the time, therefore, the electronic configuration of an atom or ion is in the ground state.

When atoms are brought together to form a solid in such models, the atoms have definite valences. When an electron hops from one atom to another, their valences change. Because the changed valence state generally has a higher energy, the atom will try to return to its most favorable valence as soon as possible. Thus in localized models we think of magnetism as being caused by well-defined magnetic moments centered on atomic sites interacting with each other by way of electrons hopping back and forth.

This picture is grounded in quantum mechanical calculations. If we examine the interaction between two atoms only, the basic mechanism is an exchange of elec-

trons between them. Thus they share magnetic information without relinquishing their states. The interaction energy of the atomic magnetic moments due to this kind of exchange can be written³ in the form

$$E = -A \mathbf{J}_1 \cdot \mathbf{J}_2$$

where each $\mathbf{J}$ is the angular momentum of that atom's electron configuration, and the magnitude *and sign* of the coefficient A depend on the details of the configurations. This interaction is called Heisenberg exchange. (See figure 1.) It has to be distinguished from the exchange energy due to the Pauli principle, but unfortunately the term "exchange interaction" is used both for the interaction between local magnetic moments and for the Pauli electron exchange.

Local magnetic-moment models are characterized by atomic correlation. The interaction between the atoms is not strong enough to destroy the atomic character of the local electronic configuration. These are very useful models for describing magnetism in materials containing rare earth or actinide atoms. They also let us calculate temperature-dependent effects. In fact, they are the natural models for discussing spin waves (magnons), even in cases where the magnetism is itinerant.

A gas of wandering electrons

In general, however, itinerant magnetism in solids, where the electrons are not bound to individual atoms, calls for a completely different approach, one based on the notion

HUND'S RULES

For the ground state of an ion with a partially filled shell, Hund's rules state that:

1. The total spin S of the system has the largest value consistent with the Pauli exclusion principle.
2. The total orbital angular momentum L has the largest value consistent with the Pauli principle and with the first rule.
3. The angular momentum vectors $\mathbf{L}$ and $\mathbf{S}$ couple antiparallel for electron shells less than half full, and parallel for shells more than half full.

of a homogeneous electron gas. If we consider a collection of electrons interacting with each other in a constant external potential, we can again calculate the properties of such a system in a completely quantum mechanical way. At low electron densities, one finds, the electron spins align in the same direction to produce magnetic order. In these models the only contribution to the magnetic moment is due to electron spins; there are no orbital moments. Just as in the case of localized magnetism, however, this magnetic order is attributable to the Pauli principle. And as before, correlation tends to decrease the amount of magnetic order.

Itinerant models are natural for describing magnetism in metals. All the core atomic electrons are, of course, very much localized. But they are all spin-paired; the filled shells contribute no net moment. Only the valence electrons contribute to the magnetism, and they are clearly itinerant. This is even true for the transition metals: Although the 3d electrons in materials like iron and nickel are spatially localized, their hopping is fast enough that one can ignore their orbital magnetic moments. Itinerant magnetism explains very well the nonintegral values of the angular momenta of 3d-transition-metal atoms in crystals.⁴

To describe the magnetic moments of the 3d transition metals one doesn't need to partition the valence electrons into localized and itinerant electrons, as older models did. Those models were based on the fact that the hopping time for the 3d electrons depends strongly on the quantum mechanical state of the electron. That dependence does, however, have important consequences when one has to choose a simple model to describe experimental results. Photoemission spectroscopy, for example, is characterized by very short interaction times and it sees all electrons as localized. Mössbauer and de Haas-van Alphen spectroscopy, on the other hand, are characterized by a long time scale; they see the 3d electrons as itinerant. Only when an experimental technique sets a time scale in the midrange of hopping times is it useful to separate the 3d electrons into localized and itinerant.

Real systems obviously do not behave exactly like either of the two classes of models I've been discussing. To improve our theory of magnetism in solids we have to combine the features of the two extreme cases. Real systems range from rare earth materials, which exhibit a localized type of magnetism, to systems like Ni_3Al , in which the magnetic order is weak and itinerant. Magnetism in the 3d transition metals is still itinerant, but it does have aspects of localization: The orbital moment does not vanish completely. Permanent magnets like NdFe_{14}B are especially hard to describe, since they combine the behavior of transition metals and rare earths.

Because we don't have a complete model of magnetism in solids, the description of real systems has to start with the simple model that works best in first approximation. Localized systems are best described by Hubbard-like models.³ The two ingredients of such models are a description of the local atomic state and a term in the Hamiltonian that corresponds to electron hopping. The latter is often included in a very approximate way, and one has to be careful in using these models for itinerant systems.

Density functional theory

A different approach to understanding the physics of

magnetic materials is offered by density functional theory.⁵ This theory includes the electron hopping in a much better approximation than do the Hubbard models. Electron exchange and correlation (the effects that lead to Hund's rules in atoms) are included in principle, but the true functional that would give the exchange-correlation energy in terms of the charge density distribution is not known.

That's where the major approximations are required in real calculations in density functional theory. The usual choice (the so-called local density approximation) is guided by the results of analytical and Monte Carlo calculations for a homogeneous, interacting electron gas. Therefore the calculations represent the itinerant limit exactly.

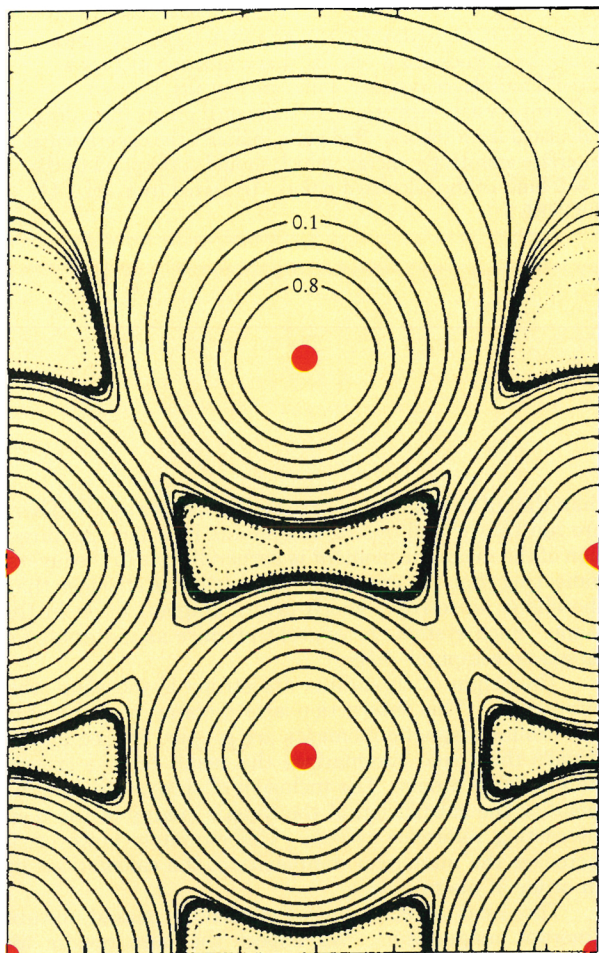
Density functional theory is based on minimization of the total energy. Thus it yields results only for the ground state of an interacting electron system at zero temperature. One could minimize the Helmholtz energy to obtain a temperature-dependent theory. But that only gives a nonzero temperature to the electron system. That excludes phonon effects. Furthermore such a formalism can only describe collective thermal behavior, not individual electronic excitations. It is, however, possible to describe spin waves and other finite-temperature effects by combining density functional calculations with localized models.⁶

The total energy of a system of interacting electrons has two components: kinetic and potential energy. In density functional theory one writes the total energy as the sum of four terms. The kinetic energy is replaced by the kinetic energy of a similar system of noninteracting electrons. The potential energy is replaced by the classical Coulomb energy of the interacting electrons plus the energy due to the nuclei and any external fields. That leaves an error term, because total energy reckoning has left out the so-called exchange-correlation energy. That's an unfortunate name, because the neglected energy is not quite the same as the exchange-correlation energy in the standard Hartree-Fock sense. In density functional theory the error term also includes a part of the kinetic energy.

All the approximations that have to be made to arrive at a useful form of the theory are related to this exchange-correlation energy. The standard procedure is the following: At each point in space the exchange-correlation properties are determined by the local charge density of interacting electrons. The exchange-correlation energy density is simply the exchange-correlation energy of a homogeneous interacting electron system with that density. Then the total exchange-correlation energy is obtained by integrating over all space.

A magnetoelectronic device consists of many atoms. Applying the Schrödinger equation directly to such a system is impossible. The first complexity reduction comes from ignoring the motion of the nuclei. Nuclear motion can be included again at the end by a collective description in terms of phonons. There are some interesting questions related to the interaction between phonons and magnetism, but I will ignore them here. I will also ignore the very small magnetic moments of the nuclei.

A magnetoelectronic device can be modeled by a unit cell of atoms that is repeated periodically throughout a lattice. The simplest Co-Pd multilayer system can be described by a unit cell with only two atoms, but the



ELECTRONIC SPIN DENSITY contour map, calculated for a seven-layer iron surface, shows the upper half of a cross section normal to the surface. Nuclei are shown in red. Spin densities labeling contour lines are in atomic units ($\hbar$ per cubic Bohr radius); adjacent contour lines differ by a factor of 2. The calculation assumes there is no net orbital contribution. Therefore, in the absence of spin-orbit coupling, the ferromagnetization direction is arbitrary. Dotted lines indicate spin density in the opposite direction. The integrated net electronic spin per atom in the central layer is 2.25 $\hbar$. (Adapted from ref. 11.) **FIGURE 2**

complexity of the unit cell increases rapidly if one wants to treat effects like interface roughness. Much work has been done to speed up density functional calculations.⁷

Results of local density calculations

The local density approximation is exact for a homogeneous electron gas. So the theory works very well for simple metals in which all bonding characteristics are determined by free electrons. Comparisons between calculated and experimental lattice constants of simple metals consistently show differences of less than 1%. From a theorist's perspective that's good agreement. One wants the theoretical errors to be smaller than typical differences in lattice constants between materials or between modifications of the same material. Local density calculations have also been very successful in determining the dependence of crystal structure on pressure.

It is somewhat surprising that local density calculations also give very good results for semiconductors and transition metals. For example, a new phase transition in silicon under pressure was predicted by such methods and later confirmed by experiment.⁸ For transition metals with nonmagnetic ground states, the errors in the calculations are similar to those for simple metals. The errors are somewhat larger for the 3d transition metals with magnetically ordered ground states. There the error in the lattice constant is typically 3%.

Magnetism plays an important role in determining the crystal structure of the ground state. If, for example, we treat iron as a paramagnetic (rather than ferromag-

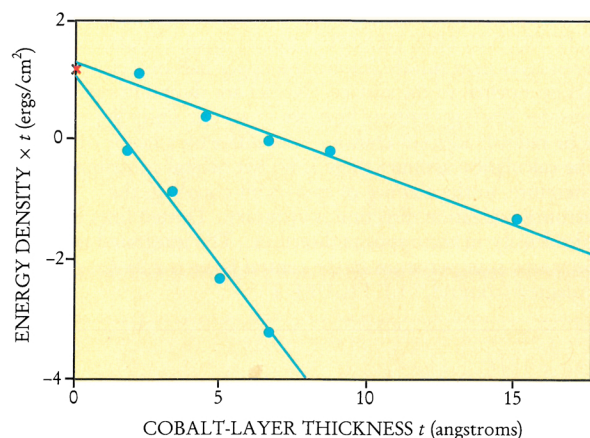
netic) system, the ground state comes out with the wrong symmetry (face-centered cubic instead of body-centered cubic) and the equilibrium density of the bcc phase is much too high. If we let magnetic order develop, the bcc phase acquires a large ferromagnetic moment, while the fcc phase becomes slightly antiferromagnetic. The bcc equilibrium density and magnetic moment are then much closer to the experimental values. The total energies of the bcc and fcc phases are almost the same, but even the best local density approximation wrongly gives the fcc phase the lower energy.⁹ Only after improving the exchange-correlation energy by adding gradient corrections to the exchange-correlation energy does one find that the ground state of the iron crystal is indeed bcc.¹⁰

In contrast with the models of localized magnetism, which are based on model Hamiltonians with free parameters, density functional calculations involve no arbitrary parameters. Once the choice of exchange-correlation potential is made, the calculations are truly *ab initio*, that is to say, from first principles. In the local density calculation one includes all effects of electron exchange and correlation present in a homogeneous electron gas. Therefore these calculations are very well suited for describing itinerant magnetism. They correctly yield, for example, the nonintegral spins of the 3d transition metals.

Figure 2 represents the electronic spin density near the surface of iron.¹¹ This contour diagram shows very clearly the high spin density near each nucleus. That's from the 3d shell of the iron atom, and it explains why magnons can be treated in a localized model, even for itinerant magnets. In the ground state of this quintessential ferromagnetic material the spin moments on all the atoms point in the same direction, which is arbitrary in the absence of spin-orbit coupling. In excited states they can point in different directions, but the spin density remains spatially localized in the 3d shell. Integrating the spin density in figure 2 shows that the magnetic moment is largest at the surface. That's a common feature of transition metals, related to the smaller number of nearest neighbors at the surface.

Although density functional calculations within the local density approximation give good results for the magnetic moments of the 3d transition metals, they fail in describing the magnetic moments in the rare earths. Electron exchange and correlation are very important in the rare earths, and the total magnetic moment has both spin and orbital contributions. The exchange and correlation effects leading to spin pairing are much the same in atoms and in the homogeneous electron gases. Both are related to the Pauli-principle tendency of electrons to avoid each other when their spins point in the same direction. Thus Hund's first rule is to some extent built into the local density approximation.

Hund's second rule dictates how the orbital moment is determined in atomic ground states. It involves the



THEORETICAL ANISOTROPY ENERGY DENSITY times cobalt-layer thickness t , calculated as a function of t for a Co-Pd multilayer system. Lines are best fits, for two different crystal orientations, to individual points (blue dots) calculated from theory. Red cross indicates the experimental interface anisotropy energy, which should correspond to the $t = 0$ limit of the calculated points. (Adapted from ref. 14.)

FIGURE 3

correlation of different orbital states. That is clearly a nonlocal effect: The orbital state is characterized by the rotational properties of the electronic wavefunction about the nucleus. In other words, one needs to know the charge density of the electrons around the nucleus, and not just at the single point in question. This part of the exchange-correlation energy cannot be derived from the homogeneous electron-gas picture. Because it is homogeneous and unbounded, the electron gas would always have zero angular momentum. The correlation needed here is atomic. Including such atomic effects will bridge the gap between the localized models and density functional theory. That is now the focus of my research.

Such correlation effects also depend on the electron density distribution around the atom. They are very hard to recover in expansions of the exchange-correlation energy in terms of gradients; such expansions converge slowly. Therefore extensions of the local density approximation that only include the lowest-order gradients are not useful for getting at Hund's second rule.

Magnetic anisotropy

As a rule one can say that for any system, like the 3d transition metals, in which the orbital magnetic moment is much smaller than the spin magnetic moment, the local density approximation gives good results for the magnitude of the spin moment. But the magnitude of the magnetic moment is not the only important issue. Its direction is often even more important for technological applications. Magnetic anisotropy is what determines how the energy of a system varies when the direction of the magnetic moment changes.

An important determinant of magnetic anisotropy is the shape of the sample. That issue can be treated as a purely classical effect completely describable by Maxwell's equations, but it also follows from the exact microscopic theory.¹² Because of the discontinuity at a surface, the shape of the sample can determine the direction of the magnetic moment. A rod, for example, has two preferred orientations of the magnetization. In a disk the magnetic moment lies in the plane of the disk. Because a perfectly spherical piece of material has, by definition, no shape anisotropy, the direction of its magnetic moment is classically undetermined.

Microscopically there are, of course, no perfectly spherical samples. The local arrangement of the atoms produces an additional term in the anisotropy. Crystalline anisotropy determines the interaction between the direction of the magnetic moment and the local atomic environment. The energy involved is normally much smaller

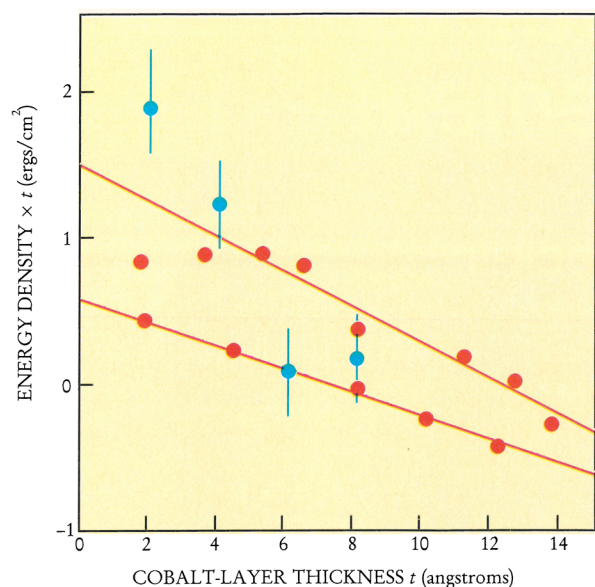
than that of the shape anisotropy, but not always.¹³ There are multilayer and overlayer systems in which the direction of the magnetic moment is perpendicular to the layers, indicating that the crystalline anisotropy is stronger than the shape anisotropy, which favors magnetization in the plane. Such systems have great promise as materials for magnetic computer disks.

The origin of crystalline anisotropy is the spin-orbit interaction. This interaction also dictates how the spin and orbital magnetic moments are coupled in free atoms. Hund's third rule summarizes the result for the ground states of free atoms. The inclusion of spin-orbit coupling modifies the calculation of the kinetic energy of the non-interacting reference system. Unfortunately however, it increases the numerical complexity of the calculations by an order of magnitude.

The local density approximation is geared toward itinerant magnetism. We expect the best results for magnetic anisotropy from systems where the orbital moment is very small. A standard theorem of atomic physics tells us that the orbital angular momentum is zero when the ground state is nondegenerate and no external magnetic field is present.³ Because a free atom is in a rotationally symmetric environment, it is degenerate, and therefore its orbital angular momentum is often large, as predicted by Hund's second rule. But if we bring free atoms together to form a crystal, the symmetry is lowered and consequently the degeneracy is decreased. That has important consequences as soon as the interaction energy is comparable to the energy splitting of the atomic multiplet states: The orbital angular momentum becomes smaller and smaller as we bring the atoms together; it is quenched. That's when the local density approximation works best. The 3d transition metals are in that regime; the rare earth materials are not.

Multilayer systems yield the best results for *ab initio* calculations of magnetic anisotropy. They also exhibit larger anisotropies. Much work has focused on Co-Pd multilayer systems. Such calculations correctly describe the perpendicular orientation of the anisotropy, and they reproduce reasonably well the dependence of the anisotropy energy on layer thickness.^{14,15} (See figures 3 and 4.) These results are actually quite remarkable, considering how small the energy differences are. The calculations have to be done with great care, but the state of the art is good enough to yield results that really help us understand the experimental data and point the way to new experiments.

For bulk materials such as iron, nickel and cobalt, on the other hand, the calculation of magnetic anisotropy



MEASURED ANISOTROPY ENERGY DENSITY times cobalt-layer thickness t in a Co-Pd multilayer system (red data points and empirical fitted lines) is plotted against t . Blue points and their error bars indicate *ab initio* theoretical calculations and their uncertainties. Upper and lower data sets are for multilayers fabricated by deposition at different temperatures. (Adapted from ref. 15.) **FIGURE 4**

constants has not been very successful. They often differ from the measured constants by orders of magnitude, and even the sign is wrong half the time. Part of the problem is numerical: The necessary Brillouin-zone integrations are much more difficult in three dimensions than in two. But there's also an important analytical problem related to the local density approximation.

The local density calculations of the magnetic anisotropy describe the spin magnetic moment quite well. If you ignore the spin-orbit coupling in the kinetic energy, the calculations do not give any orbital magnetic moment, because there are no terms in the exchange-correlation energy that generate orbital angular momentum. Including spin-orbit coupling changes this picture. Now the spin moment produces orbital angular momentum, which couples to the spatial directions in the crystal. By varying the direction of the spin moment one can measure the change in total energy and thus get the magnetic anisotropy energy. In this approach the spin-orbit coupling both causes the orbital magnetic moment and couples it to the spin moment.

That's clearly the wrong mechanism for rare earth materials. There the orbital angular momentum is driven by electronic exchange and correlation, mainly through the Pauli principle. Thus there have to be additional terms, of atomic character, in the exchange-correlation energy. With these extra terms in density functional calculations we can get a much improved description of rare earth materials. Approximate calculations along these lines have demonstrated the importance of such corrections, and they illustrate the difficulties of describing magnetic anisotropy in rare earth systems and bulk transition metals by the local-density approximation.¹⁶

Electronic-structure calculations for itinerant systems are very promising. They have been especially successful at surfaces and interfaces. It is now possible to describe the strain in metallic multilayers in terms of the total energy, and one can predict the structure of overlayers. Even calculations of the magnetic anisotropy for multilayers are now reliable, because correlation effects are small in these low-dimensional systems. In principle, theoretical calculations can now predict in which systems one will find perpendicular anisotropy.

Challenges for the future include modeling itinerant systems with structure corresponding to the imperfections of real samples.¹⁷ In such work one has to consider unit cells containing many atoms. That will require faster calculational techniques. We also want to understand magnetic anisotropy in rare earths and bulk transition metals. For that we will need a better description of exchange-correlation effects in density functional theory and how they generate orbital magnetic moments.

In this article I have only addressed ground-state properties of magnetic systems. Transport phenomena fall outside this domain. But an understanding of spin-polarized transport, the subject of the article by Gary Prinz on page 58, must start from a good description of the ground state of itinerant magnets.

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