

# **Small polarons**

Excess charges trap themselves in solids or liquids by shifting the surrounding atoms, yielding entities whose behavior sheds light on phenomena ranging from charge solvation to photocarrier survival.

## David Emin

We usually think of electrons in solids and liquids as behaving like free particles whose motion is impeded by occasional collisions. Evidence is now accumulating for charge carriers with qualitatively different behavior. These new charge carriers, in the simplest case, are extra electrons in condensed matter that become trapped in potential wells of their own creation, forming units known as small polarons.

In the last few years, experimental and theoretical research on small polarons has intensified. The results of this work are contributing to our understanding of a wide range of phenomena, including, for example, the diffusion of light atoms through metals, the solvation of electrons in liquids, and the nonradiative recombination of electrons and holes in semiconductors and insulators.

A small polaron is an extra electron or a hole severely localized within a potential well that it creates by displacing the atoms that surround it. Injected electrons in liquid ammonia, for example, solvate by forming small polarons, which provide the blue hue in figure 1. We call a polaron "small" when the spatial extent of the wavefunction of the excess electron or the hole is less than or comparable to the separation of the atoms or molecules. The charge carrier then moves only in response to appropriate motions of the surrounding atoms. (Large polarons have somewhat different properties, and, although not the subject of this article, are themselves the object of much research.)

It has been almost 50 years since Lev Davidovich Landau set forth<sup>1</sup> the notion of the small polaron. Nonetheless, it is recent years that have seen the most rapid accumulation of evidence of small polarons and the most rapid development of the theory.

There is now evidence that small polarons exist in alkali halides, some transition-metal oxides (see A. Marshall Stoneham's article in Physics Today, January 1980, page 34), rare-gas solids, molecular crystals and various glasses. While it is generally accepted that the charge carriers in glasses containing transition-metal ions and the holes in amorphous silicon dioxide form small polarons, the issue remains a subject of debate for the chalcogenide glasses and other amorphous semiconductors (see the article by Jan Tauc in Physics Today, October 1976, page 23).

Small-polaron theory envisions a charge carrier in a semiconductor or insulator. However, the theory applies generally to a particle or a quasiparticle interacting with relatively massive atoms surrounding it. For example, replacing the electron or hole of small-

Extra electrons in liquid ammonia form small polarons, which appear blue. Each solvated electron resides in a potential well produced by the orienting of ammonia molecules that surround it. The polaron is the entire unit made up of the self-trapped carrier and the pattern of orientation of the surrounding molecules. (Photograph courtesy of Karl I. Trappe and James C. Thompson, University of Texas, Austin).

polaron theory with an exciton—an electron bound to a hole—one obtains the theory of the formation and motion of self-trapped excitons. With modifications the theory also applies to:

- ▶ diffusion in metals of light interstitial atoms such as hydrogen and its isotopes
- ▶ solvation of electric charges in li-
- phonon-assisted hopping of charge carriers in semiconductors and insulators
- nonradiative recombination in semiconductors and insulators, and
- ▶ the capture and release of charge carriers from severely localized, or "deep," polaronic traps, also in nonmetals.

The properties of small polarons are often opposite those of quasifree charge carriers. Because of its connection with surrounding atoms, a small polaron has a mobility of less than 1 cm<sup>2</sup>/ V sec, which is very much lower than that generally associated with quasifree motion. And while the mobility of a quasifree carrier typically falls with increasing temperature, small-polaron mobility usually increases with temperature. The Hall effect and the frequency dependence of the mobility also differ qualitatively from those of quasifree charge carriers. In fact, even the sense in which a magnetic field deflects a small polaron can be opposite to that of a similarly charged free particle. In this situation a small polaron circulates in a magnetic field in the same direction as an oppositely charged free particle. Interactions between small polarons can also differ significantly from those of free particles. Namely, like-charged small polarons may experience a short-range attraction, and oppositely charged small polarons can exhibit a short-range repulsion. It is the challenge of predicting and observing such distinctive properties that has spurred interest in small polarons.

In this article we will look at the basic principles that govern the formation and motion of small polarons.

### Small-polaron characteristics

What are the consequences of placing a stationary excess electronic charge within a solid? The atoms that surround the stationary carrier will experience an additional Coulomb force, which will alter their equilibri-

um positions (figure 2). These atomic displacements are such as to lower the potential energy of the excess charge. If the potential well produced by the atomic displacement pattern is sufficiently deep, the carrier may occupy a bound state. In this circumstance the excess charge cannot escape from its position in the solid without an alteration of the positions of the surrounding atoms. Because the potential well that binds the carrier arises from atomic displacements caused by the carrier's presence, the carrier is said to be self-trapped.

The polaron is the entire unit comprising the self-trapped carrier and the atomic-displacement pattern. In the case of a small polaron in a simple inorganic solid—a hole in KCl, for example—the characteristic radius of the self-trapped carrier is less than or comparable to an interatomic separation. As we mentioned earlier, we call such polarons "small."

An electron, be it self-trapped or not, can equally well reside at any of the geometrically equivalent sites of a crystal. Just as the partial lifting of this translational degeneracy gives rise to a band of Bloch eigenstates for quasifree electrons, so, in the case of a small polaron, Bloch-like small-polaron eigenstates result.2 In either situation the width of the energy band in a tightbinding scheme is proportional to the energy associated with transposing the carrier (quasifree electron or small polaron) between identical local states centered at adjacent, topologically equivalent crystal sites.

However, for a small polaron this transfer energy is typically many orders of magnitude smaller than it is for an electron. The reason for this difference is that transposing a small polaron requires transferring not only the self-trapped electron but its atomic displacement pattern as well. The latter component involves the quantummechanical tunneling of the atoms comprising the small-polaronic displacement pattern; the atoms tunnel between two different displacement patterns. Because a number of these atoms would have to tunnel distances that are much larger than the decay lengths of the atoms' wavefunctions, such motion is relatively rare. Thus the transposition of the displacement pattern is characterized by a very small transfer energy, and the transfer is slow. That is, the small polaron is typified by a very narrow bandwidthmuch less than one meV.

I should stress here that the term "polaron" is an unfortunate misnomer. The term was coined as an outgrowth of early considerations of self-trapping in polar and ionic solids. In these materials the charge carrier interacts with the long-range dipolar polarization field as-

sociated with the relative displacement of different types of atoms, such as the anions and the cations of an ionic lattice. Such displacements are characteristic of optic- and polar-mode lattice vibrations. However, self-trapping is not at all restricted to polar and ionic materials with a long-range dipolar component of the electron-lattice interaction. In fact, in most instances of small-polaron formation it is the short-range component of the electron-lattice interaction that plays the major role. Here, the energy of a carrier depends primarily upon the displacements of neighboring atoms. Thus, self-trapping occurs in covalent as well as polar and ionic materials. And it generally involves the interaction of the carrier with acoustic as well as optic vibrational modes.

### Formation of small polarons

In what follows we will assume that an excess charge has a short-range interaction with the atoms of a solid. That is, we presume that the energy of an electron depends only on the displacements of atoms in its neighborhood. A short-range electron-lattice interaction allows only two qualitatively distinct types of groundstates for an excess electron in a deformable solid. 3-5 Either the charge carrier remains unbound or it self-traps to form a small polaron.

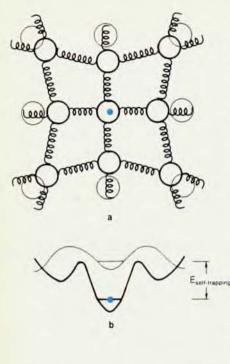
To understand the origin of this dichotomy, first consider the analogous situation of an electron in an isotropic elastic continuum. <sup>5,6</sup> Here the potential energy of the electron varies linearly with the deformation, or "dilatation," of the continuum at its location. Noting that the electron is very much lighter than the atoms of the material, we employ the adiabatic approximation. That is, we consider the electron's energy to be a function of the static deformational configuration of the continuum.

There are three contributions to the system's energy: the electron's kinetic and potential energies and the elastic energy required to strain the continuum. By minimizing the sum of these energies with respect to dilatation we get<sup>5,6</sup> an expression for the ground state dilatation of the system:

$$\Delta(r) = -Z/S|\Psi(r)|^2$$

Here Z is the energy characterizing the strength of the electron-continuum interaction (analogous to the deformation potential constant), S is the stiffness coefficient of the elastic continuum and  $\Psi(r)$  is the electron's wavefunction. Thus dilatation increases with the interaction strength, decreases with the material's stiffness

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Small-polaron level Small-polaron band

Polaron formation, electron energy and polaron energy. a: Excess electron (dot) displaces lattice atoms (circles), forming a polaron. b: Displaced atoms provide a potential well (dark curve) that differs from that produced by undisplaced atoms (light curve). The electron's energy decreases by the self-trapping energy. c: The polaron has less energy than does an electron in a perfectly rigid solid. The energy of the polaron is lower by its binding energy  $E_b$ , which is the difference between the self-trapping energy and the strain energy associated with deforming the lattice.

and mirrors the electron's density distribution.

At an energy minimum, the stationary wave equation

$$[-(\hbar^2/2m)\nabla^2 + Z\Delta(r)]\Psi(r) = E\Psi(r)$$

becomes the nonlinear differential equation

$$[-(\hbar^2/2m)\nabla^2 - (Z^2/S)|\Psi(r)|^2]\Psi(r) = E\Psi(r)$$

This equation, analogous to those for solitons, admits localized as well as nonlocalized solutions.

For example, with the electron's density spread uniformly over an arbitrarily large volume V, the interaction term is negligible because  $|\Psi(r)|^2$  is proportional to 1/V, and the electron is essentially free. However, solutions for which the electron is localized (self-trapped) are also possible.

The small-polaron solution. We can readily use a scaling argument to extract the essential features of the ground-state solutions of the eigenvalue equation.  $^{5,6}$  Noting that the ground state solution for an isotropic system is spherically symmetric, we write the energy E of the system as a function of a single scaling parameter R, which is related to the spatial extent of the electron's wavefunction. In particular, for a well-behaved eigenstate of finite radius, the true ground-state energy, the minimum of E(R), occurs at R=1. It turns out that

$$\begin{split} E(R) &= T_{\rm e}/R^2 - V_{\rm int}/R^d + E_{\rm strain}/R^d \\ &= T_{\rm e}/R^2 - V_{\rm int}/2R^d \end{split}$$

where  $T_{\rm e}$  and  $V_{\rm int}$  are constants respectively related to the electron's kinetic and potential energies, and d is the dimensionality of the continuum. We have used  $E_{\rm strain} = {}^{1}\!\!/_{2}V_{\rm int}$ , which is valid when the electron's potential energy varies linearly with the dilatation.

As figure 3a shows, for a one-dimensional continuum, E(R) possesses a minimum at a finite radius. However, for a three-dimensional system there are two relative minima. The minimum at  $R=\infty$  corresponds to a free electron in an unstrained continuum—analogous to a conduction-band state. The minimum at R=0 corresponds to an electron bound in an infinitely deep well of infinitesimal extent—the continuum version of a small polaron.

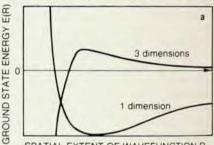
The two minima are separated by an energy barrier. Thus, to pass adiabatically between nonpolaronic  $(R=\omega)$  and small-polaronic (R=0) states requires a change in deformation parameters. This occurs only when energy is supplied to the system—going over the barrier—or when the atoms of the continuum tunnel quantum-mechanically between different deformational configurations—passing through the energy barrier.

By way of contrast, in the one-dimensional system there is no such impediment to a free charge forming a polaron.5,6 There a charge will displace the atoms surrounding it in a time of the order of an atom's vibrational period, about a picosecond. With such a temporal measure in mind, researchers speak of the energy barrier in the three-dimensional system as creating a "time delay for self-trapping." Here one pictures an injected charge wandering quasifreely through a solid until it encounters a situation in which the atoms surrounding it have assumed a configuration that is suitably deformed so that relaxation to the self-trapped state proceeds without impediment.

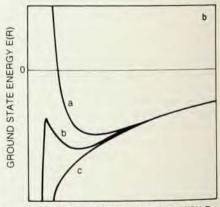
The fact that the small-polaron state (at R=0) is always lower in energy than the nonpolaronic state (at  $R=\infty$ ) is an artifact of the continuum model. Actually, in a simple monatomic discrete system the electron–lattice interaction saturates as the radius of the self-trapped electron shrinks to less

than an interatomic separation. If we incorporate this feature into the continuum model, then E(R) cuts off when R is less than a critical radius  $R_c$ , which is comparable to an interatomic distance. With the cut-off at a smaller value of R than that of the peak of E(R) (see figure 3a), the small-polaron state is either metastable,  $E(R_c) > E(\infty)$ , or stable,  $E(R_c) < E(\infty)$ .

Effect of defects. The electron-continuum interaction can act synergistically with the localizing potentials associated with defects to produce small-polaronic localized states.6 Consider, for example, an electron in a deformable continuum in the presence of a positively charged defect (figure 3b). Without any electron-continuum interaction there is a single finite-radius (hydrogenic) minimum associated with an electron in the defect's Coulombic well (curve a). However, with a finite electron-continuum interaction, a severely localized small-polaronic defect may form (curve b). The dichotomy between large-radius weakly polaronic defect states and small-polaronic defect states is analogous to that between nonpolaronic and small-polaronic states in a defect-free continuum. However, when the attractive potential of the defect, and the electron-continuum interaction are both of sufficient strength, the



SPATIAL EXTENT OF WAVEFUNCTION R



SPATIAL EXTENT OF WAVEFUNCTION R

Ground-state energy of a system consisting of an electron in a deformable continuum depends on the spatial extent of the electron's wave function. a: Electron in one- and three-dimensional continuum b: Electron in a three-dimensional continuum with a positively charged defect. Energy is plotted for three successively greater strengths of electron-continuum interaction (a, b and c).<sup>6</sup> Figure 3

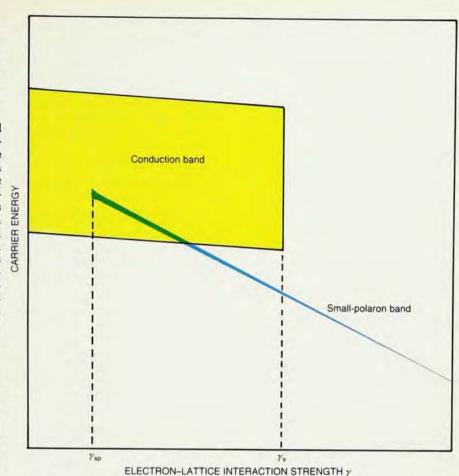
barrier to the small-polaronic state is eliminated, as in curve c, and only the small-polaronic defect state survives. Thus, the localizing potentials of defects generally reduce, and sometimes destroy, the barrier to self-trapping, thereby enhancing the likelihood that small polarons will form.

Theoretical physicists have carried out variational studies beyond the adiabatic approximation to determine the eigenstates of an excess electron in a deformable crystal.4.5 Here the atomic deformation pattern is no longer constrained to be static. Figure 4 depicts schematically the situations in which dynamically stable nonpolaronic and small-polaronic carriers can exist in such a crystal. The carrier's energy is plotted against the electron-lattice interaction strength γ, which is proportional to the small-polaron binding energy. Increasing  $\gamma$  may be thought of as placing the electron in progressively softer, more deformable, materials. From this point of view, the very narrow band of small-polaronic states exists only for sufficiently soft materials—those having  $\gamma > \gamma_{sp}$  (figure 4). In these materials a small polaron forms when the electron causes a substantial displacement of the surrounding atoms and is self trapped. The relatively wide bands of nonpolaronic states, the usual conduction-band states of a semiconductor or insulator, exist only for sufficiently stiff materials-those for which  $\gamma < \gamma_s$ . In these stiff materials the presence of the carrier induces only minimal changes in the positions of the lattice atoms.

For sufficiently weak electron-lattice coupling, characterized by  $\gamma < \gamma_{sp}$ , a small polaron is unstable and will decompose. For  $\gamma > \gamma_s$  the nonpolaronic electron is dynamically unstable and will collapse to a small polaron. That is, in such soft materials the electron cannot move between atomic sites fast enough to preclude inducing significant displacements of the atoms surrounding it. It collapses to a small polaron much as a pebble skimming a pond sinks when it slows. Consistent with the adiabatic approximation of a three-dimensional continuum, in the adiabatic limit for a lattice,  $\gamma_s \rightarrow \infty$ and  $\gamma_{sp} \rightarrow 0$  so that both nonpolaronic and small-polaronic states coexist for all values of the electron-lattice coupling strength y. Thus we understand the conditions under which a charge carrier self-traps and forms a small polaron as well as the conditions under which it remains nonpolaronic.

### Small-polaron hopping

There is uncertainty in the small polaron's energy because of scattering events and site-to-site variations in the potential energy associated with defects and disorder. This uncertainty



**Energy bands** as a function of crystal stiffness. Schematic diagram shows the lowest-lying energy levels available to an electron in a 3-dimensional insulator. Crystal lattices become more deformable—less stiff—as one moves to the right on the horizontal axis.<sup>5</sup> Figure 4

often greatly exceeds the width of the small-polaron band, which is extremely narrow. As a result, the polaron's motion is usually described as proceeding via a succession of phonon-assisted hopping events.<sup>2</sup>

Figure 5 shows the steps that may be involved in a single hop. The two frames at the bottom of the figure depict the atomic displacement patterns and potential wells for a small polaron located at each of two equivalent adjacent lattice sites. The direct motion of the small polaron between equivalent sites is related to small-polaron banding and involves a single step (path a). Here the electron and the equilibrium deformation pattern concurrently tunnel between the two situations.

In addition to direct motion, hopping occurs indirectly, in what we can think of as a three-stage process.

▶ First, amidst random oscillations about their equilibrium positions, lattice atoms in the vicinity of the electron assume a distortion pattern that is associated with a greater transfer rate than that of the equilibrium distortion pattern. Here the disparity between the two deformation patterns involved in the transfer of the electron is less

than the disparity between their equilibrium configurations. Such an atomic configuration comes about through the transient concentration of vibrational energy in the vicinity of the electron.

 Second, the electron moves between degenerate electronic energy levels. Transient deformation patterns that involve relatively small local concentrations of vibrational energy differ only slightly from those of the ground state. So the transfer rate is still reduced by the incomplete overlap of initial and final atomic displacement patterns (path b). However, with a greater concentration of vibrational energy, it is possible to have deformation patterns between which an electron can transfer without bringing about further deformation (path c). The occurrence of such a configuration of lattice atoms, for which the electronic energies associated with the initial and final sites are equal, is termed a "coincidence event." We speak of electronic hops involving coincidence events as semiclassical because tunneling of the atomic deformation pattern does not play a significant role.

▶ Third, after the electron transfers between sites, the local deformation pattern relaxes, dissipating the distortional energy to the material as a whole

Jumping rate. Figure 6 is a representative plot of the small-polaron jump rate as a function of reciprocal temperature, measured in units of  $\theta$ , a temperature characteristic of the atomic vibrations. For acoustic phonons,  $\theta$ is of the order of the Debye temperature. At low temperatures  $(T \leqslant \theta)$  the jump rate is nonexponential, that is, it does not obey Arrhenius's law. In this nonexponential region, increasing temperatures bring into play higher-energy processes, which involve progressively more overlap between initial and final atomic displacement patterns. These processes contribute increasingly to the jump rate.

At sufficiently high temperatures

 $(T \gtrsim \theta)$  the atomic overlap is essentially unity, because the predominant mechanisms of transfer are semiclassical. The jump rate R is then simply thermally activated. Its activation energy  $E_{\rm A}$  is the minimum energy required to deform the equilibrium configuration so as to allow a coincidence event. Explicitly, in the high-temperature semiclassical regime

$$R = [v \exp(-E_A/kT)]P$$

where  $\nu$  is the characteristic atomic vibrational frequency,  $k\theta/h$ . The term in square brackets in the equation represents the rate at which a carrier experiences coincidence events. The final factor, P, is the probability that an electron will respond rapidly enough to the occurrence of a coincidence event so as to negotiate a hop.<sup>2</sup>

C A c a Initial Final

Hopping of an electron-based small polaron. The trapped electron hops by following changes in the displacement pattern of the surrounding atoms. The short lines depict the lattice displacement pattern by connecting the position of each atom with the position it would have in a carrier-free lattice. Black dots represent atoms; red dots represent electrons or atoms with an extra electron. Potential wells and electron energy levels appear below the associated displacement patterns. Three hopping mechanisms are shown: a, direct motion; b, low-temperature hopping; c, high-temperature (semiclassical) hopping.

The time required for an electron to move between coincident levels varies inversely as the transfer energy, which is proportional to the energy splitting associated with the degenerate electronic levels of a coincidence event. For sufficiently large transfer energies the electron can always adjust to the atomic motion and move between sites: the hops are then termed adiabatic and  $P \approx 1$ . Alternatively, when the transfer energy is small the electron has only a limited ability to follow the atomic motion. We refer to these hops as nonadiabatic, and P is both much less than unity and proportional to the square of the transfer energy.

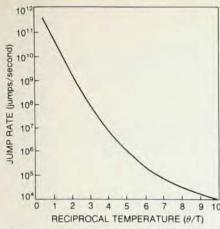
We can generalize the theory of phonon-assisted hops between equivalent states at equivalent sites to include phonon-assisted transitions between inequivalent states. The results apply to many problems including electron hopping in disordered materials, the capture and release of carriers by traps, nonradiative recombination, photon-assisted hopping and hopping in an applied electric field.

The diffusion constant associated with the hopping of a small polaron is inversely proportional to the mean time between hops. When the mean time between hops is less than the time required for the atomic displacement pattern associated with a hop to relax, successive hops of a small polaron will be correlated.9 Then the charge will move to another site before the local vibrational excitation associated with preceding hops has dissipated. Thus, the charge finds itself surrounded by atoms of greater than usual vibrational agitation, which enhances the likelihood of a hop. The activation energy associated with such correlated hopping can be small enough that the small-polaron mobility has a very weakly temperature-dependent value of about 1 cm<sup>2</sup>/V sec. One finds this behavior in a wide variety of molecular solids (see the article by Charles Duke and Larry Schein in PHYSICS TODAY, February 1980, page 42).

## Hall effect

The motion of a small polaron in a magnetic field is qualitatively distinct from that of a nearly free charge carrier. For free charges the Hall mobility—the angular deflection of a carrier per unit magnetic field—has the same value as the drift mobility—the steady-state drift velocity of a carrier per unit electric field. Furthermore, for free charges the sign of the Hall mobility is determined solely by the sign of the carrier. For small-polaron hopping neither of these two characteristics applies in general.

To appreciate the origin of these differences, note that reversing the orientation of the magnetic field cannot



Rate of small-polaron jumping typically increases rapidly with temperature, as this typical plot shows. Reciprocal temperature is measured in units of  $\theta$ , which is on the order of the Debye temperature. <sup>6</sup> Figure 6

alter the direct motion of a charge between two sites, which is the primary mechanism underlying the drift mobility. However, the Hall mobility arises from contributions to the jump rate that involve interference between the transition amplitudes associated with various paths between initial and final sites (paths traversing one or more intermediate sites). These contributions do depend<sup>10</sup> on the sign of the magnetic field (see figure 7). Thus the Hall mobility is generally quite different from the drift mobility.

The magnetic field manifests itself in hopping motion when the atoms assume a deformation pattern that gives the carrier a choice between two equivalent final sites. Thus, for example, in the semiclassical regime, while the drift mobility is associated with the occurrence of a coincidence event involving two sites, the Hall effect is associated with the occurrence of a coincidence event involving three sites. The resulting activation energy for the Hall mobility is the difference between the energies associated with forming triple and double coincidence events, while the drift mobility activation energy is simply that of forming a double coincidence. Typically, the small-polaron Hall mobility is much less temperature-dependent than is the drift mobility.11 In fact, the Hall mobility of hopping small-polarons can even fall with rising temperature (see figure 7).

The sign of the Hall coefficient generally depends not only upon the sign of the carrier, but on the topology of the sites and the local orbitals between which the carrier moves. 12 For example, if an odd number of sites are involved, the sign of the Hall coefficient depends upon the sign of the product of the electronic transfer integrals associated with each step of the predominant interference process. The sign of

this product depends on the symmetry and topological arrangement of orbitals between which the carrier moves. In various instances the sign of the Hall coefficient is anomalous relative to that of a free carrier. For example, a magnetic field may deflect electron-based small polarons in the same direction that it deflects positively charged free particles. Researchers have seen Halleffect sign anomalies in various amorphous semiconductors, including amorphous silicon, germanium, arsenic and many chalcogenide glasses.

# Small-polaron interactions

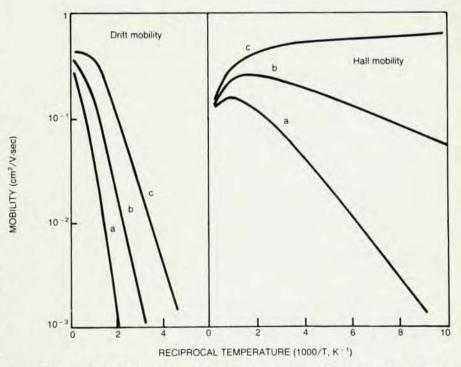
The interactions between small polarons can be markedly different from those of simple stationary charges. The reason for the difference is that, in addition to the direct Coulomb interaction between the charges, small polarons interact via the overlapping of their atomic deformation patterns.13 Consider, for example, the indirect interaction between two electrons at large separation that are each selftrapped as a result of their attraction of nearest-neighbor atoms (see the left half of figure 8). The electrons exert counteracting forces on the atoms between them. As a result, the atomic displacements associated with selftrapping are partially negated, thereby raising the energy of the pair of small polarons: At sufficiently large separations the interaction of atomic displacement patterns is repulsive.

However, as the separation between

the electrons is reduced, they increasingly act in tandem to displace an increasing number of atoms that surround them. Ultimately, when the electrons occupy the same site, the surrounding atoms are attracted by both charges. This increases the magnitude of the atomic displacements. Concomitantly the one-electron energy of each self-trapped electron is lowered, as is the total polaronic energy of the system. Thus, at sufficiently small separations the small polarons experience an attractive component in their interaction.

If this attractive interaction exceeds the Coulomb repulsion of the two electrons, the pair of negative small polarons may bind together into a bipolaron. Investigators have been using the notion of the bipolaron for several decades in an effort to understand the ground state of electrons in liquids, transition-metal oxides, organic solids and amorphous semiconductors.

Just as like-charged small polarons can experience a short-range attraction, so small polarons of opposite charge can encounter a short-range repulsion. This occurs when the forces of oppositely-charged small polarons on the atoms surrounding them are in opposite senses, as shown in the right half of figure 8. The repulsion between oppositely-charged small polarons arises through the same mechanism that produces the attraction that we have just described between like-charged small polarons. The short-



**Drift and Hall mobilities** are plotted here against reciprocal temperature for three values of the relative strength of coupling between electrons and the lattice. <sup>11</sup> Relative strengths are (a) 1.00, (b) 1.25, (c) 1.67. Figure 7

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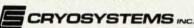
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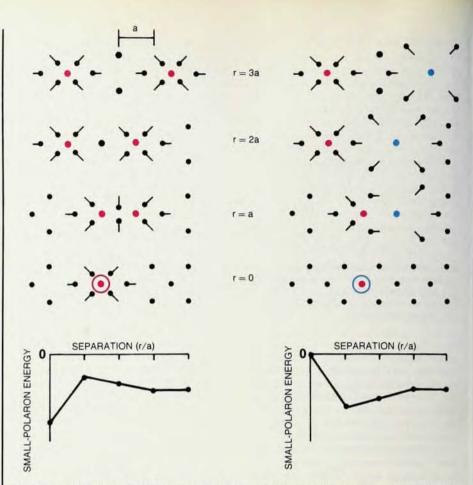
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Interactions between small polarons are attractive or repulsive depending upon the charge and separation of the polarons. The net force between two small polarons is the result of competition between the interference of their atomic displacement patterns and the Coulomb force between their charges. Symbol scheme follows that of figure 5, with blue dots representing holes. The small-polaron energies reflect only the interaction due to overlap of atomic displacement patterns; they do not include the direct coulomb interaction. Figure 8

range repulsion between electronbased and hole-based small polarons can drastically affect recombinative properties such as photocarrier lifetimes and the transient behavior of the luminescence associated with recombination.

Research on small-polaron formation and motion continues at an accelerating pace. Investigators are measuring transient optical and electrical signals to study the time delays associated with self-trapping and capture in severely localized small-polaronic traps. The circumstances in which the imposition of disorder triggers self-trapping are receiving attention. An attempt to understand the motion of carriers of intermediate mobility (about 1 cm<sup>2</sup>/V sec) has led to an extension of the theory of correlated small-polaron hopping motion. And researchers are applying small-polaron hopping theory to the mutually analogous situations of light interstitial diffusion, nonradiative recombination, trapping and phonon-assisted hopping in general. Meanwhile, data on small polarons accumulates from studies of the electronic and optical properties of crystalline and noncrystalline semiconductors, narrowband insulators, molecular solids and liquids.

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