

vin and Hopfield¹⁰ and by Onodera¹¹; conceivably these effects could also influence the $L_{2,3}$ edge shape, as could phonon and lifetime broadening. We have not analyzed the $L_{2,3}$ edge data for Mg in an effort to separate one-electron and many-electron effects because we feel such analyses may be misleading. The calculated spectra certainly exhibit spikes at the $L_{2,3}$ edges but the precision may be insufficient to permit confident extraction of accurate many-body exponents from spectra whose many-body enhancements are small to begin with. Thus we conclude that (1) one-electron band-structure effects are significant in Mg and may be significant at x-ray thresholds in other free-electron metals as well, and (2) the $L_{2,3}$ edge of Mg is a poor testing ground for many-body threshold effects.

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Electronic Structure of Amorphous Semiconductors*

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The Fermi energy as a function of electronic density and temperature is calculated for a defect level in which the effective intrasite electronic correlation energy is negative. It is found that the Fermi level lies *below* the energy of the highest-filled quasiparticle state, even at $T=0$, a result which favors p -type conduction. Furthermore, the Fermi energy varies only very slowly with electronic density and temperature, and thus is effectively pinned.

Although amorphous semiconductors exhibit as wide a range of electronic behavior as crystalline semiconductors,¹⁻³ they can be subdivided into two major classes with sharply different properties. Amorphous solids made up primarily from Group-IV or Group-V elements typically have n -type thermopower,⁴ exhibit variable-range hopping at low temperature,⁵ show an EPR signal,⁶ and have a Fermi energy which can be

moved by varying the electronic density.⁷ In contrast to this, chalcogenide glasses generally have p -type thermopower,⁴ do not exhibit variable-range hopping,¹⁻³ do not show an EPR signal,⁸ and have a Fermi energy which does not vary much with electronic density.⁹ In order to explain some of these properties, Street and Mott¹⁰ proposed a model in which the localized states in the gap of chalcogenide glasses appear at dan-

gling bonds and have a negative effective electronic correlation energy. The latter had previously been suggested by Anderson¹¹ to account for the apparent complete diamagnetism of these materials. In this Letter, some of the ramifications of a negative effective correlation energy are considered by calculating the Fermi energy as a function of electronic density and temperature within the Hubbard model.¹² The results strengthen the applicability of such a model to the chalcogenide glasses by accounting for the tendency towards *p*-type behavior, the suppression of variable-range hopping, and the apparent strong pinning of the Fermi energy which characterize these materials.

Consider a semiconductor with valence- and conduction-band edges at E_v and E_c , respectively, and with localized states in the gap arising from a single defect at energy T_0 . It is assumed that $E_c - T_0$ and $T_0 - E_v$ are always large com-

pared to kT . If U represents the effective electrostatic attraction that exists when two electrons (one of each spin) are simultaneously present in the vicinity of the same defect, then the appropriate Hamiltonian is

$$H = T_0 \sum_{i,\sigma} n_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $n_{i\sigma}$ is the number operator for electrons with spin σ localized on the defect at site i . The eigenvalues of this Hamiltonian are

$$E_m = NT_0 - mU, \quad (2)$$

where N is the total number of electrons associated with the defect states and m is the number of doubly occupied sites.

Consider a particular defect site. It is either completely unoccupied ($E=0$, nondegenerate), singly occupied ($E=T_0$, twofold degenerate), or doubly occupied ($E=2T_0-U$, nondegenerate). The grand partition function for N_0 defects is thus

$$Z = [1 + 2 \exp[-(T_0 - \epsilon_F)/kT] + \exp[-(2T_0 - U - 2\epsilon_F)/kT]]^{N_0}, \quad (3)$$

where ϵ_F is the Fermi energy and T is the temperature. The average number of electrons per defect site, $n = N/N_0$, is then

$$n(\epsilon_F, T) = \frac{1}{N_0} kT \left(\frac{\partial \ln Z}{\partial \epsilon_F} \right)_T = \frac{2 \{ \exp[-(T_0 - \epsilon_F)/kT] + \exp[-(2T_0 - U - 2\epsilon_F)/kT] \}}{1 + 2 \exp[-(T_0 - \epsilon_F)/kT] + \exp[-(2T_0 - U - 2\epsilon_F)/kT]}. \quad (4)$$

Equation (4) can be inverted to solve for the Fermi energy as a function of electronic concentration and temperature. The result is

$$\epsilon_F = T_0 - kT \ln \{ (n^{-1} - 1) + [(n^{-1} - 1)^2 + (2n^{-1} - 1)e^{U/kT}]^{1/2} \}. \quad (5)$$

For low temperatures, $kT \ll U$, and Eq. (5) becomes

$$\epsilon_F \approx T_0 - \frac{1}{2}U - \frac{1}{2}kT \ln(2n^{-1} - 1). \quad (6)$$

This is expected to be a good approximation for most chalcogenide glasses, in which U can be estimated to be of the order of 0.5 eV.¹³

There are several very interesting features of (6). For the case of exactly one electron per defect, $n=1$, and

$$\epsilon_F = T_0 - \frac{1}{2}U, \quad (7)$$

independent of temperature. More important, for any electronic density, the Fermi energy is given by (7) in the limit of zero temperature. For $n > 1$, ϵ_F slowly increases with increasing temperature, while for $n < 1$, ϵ_F slowly decreases with increasing temperature. But in any event, *the Fermi energy does not vary much with electronic density.* This provides a natural explanation of the fact that field-effect measurements in-

dicates a very large density of states at ϵ_F in chalcogenide glasses, but no variable-range hopping is observed. As electrons are injected into this system, they populate the quasiparticle levels at T_0 and $T_0 - U$, leaving the Fermi energy unchanged. However, there is actually no density of quasiparticle states at ϵ_F ; the Fermi energy is pinned by states $\pm \frac{1}{2}U$ away.

Perhaps the most nonintuitive result of this calculation is that the Fermi energy lies *below* the energy of the highest filled one-electron state, even at $T=0$. This does *not* occur when $U < 0$,¹⁴ and so is not due simply to the introduction of electronic correlations. In fact, it is the only system to our knowledge for which ϵ_F is not halfway between the highest filled and the lowest empty quasiparticle states at $T=0$. The physical reason for this apparently strange result is that although excitation of one electron from the valence band to the defect state requires

an energy of $T_0 - E_v$, excitation of *two* electrons takes an energy of only $2T_0 - U - 2E_v$. Thus, excitation of a large number of electrons requires an *average* energy of $T_0 - U/2 - E_v$ or $\epsilon_F - E_v$, as it should. The physical consequence of this result is that ϵ_F is lower in energy than would be expected from the defect energy T_0 . Consequently, ϵ_F is closer to the valence band than it would be for positive or zero electronic correlation energy, and *p*-type conduction is favored. This is in agreement with experimental results on chalcogenide glasses, almost all of which exhibit a *p*-type thermopower.¹⁻⁴

The results are quite different for positive electronic correlation energy.¹⁴ In this case, the Fermi level lies at T_0 for $n < 1$ and at $T_0 + U$ for $n > 1$, as would be naively expected. There is a finite density of one-electron states at the Fermi energy and ϵ_F moves considerably with increasing temperature (except for the particular values $n = \frac{2}{3}, 1$, and $\frac{4}{3}$). These results are consistent with the observation of a modulation of the Fermi

level via a variation of electronic density and with the predominance of variable-range hopping near ϵ_F at low temperatures. We can conclude from the experimental data^{5,7} that materials such as amorphous Si indeed have a positive correlation energy. Figure 1 shows the variation of ϵ_F with n at a given temperature for the cases of both a positive and a negative correlation energy. The relative pinning of ϵ_F in the latter situation is clear.

The densities of quasiparticle states for the cases of both positive and negative electronic correlation energies are sketched in Fig. 2 for several values of the electronic density. Possible optical transitions are indicated. For positive correlation energy, except for the special case $n = 1$, three optical transitions connecting localized and extended states are possible. The sum of two of these should be equal to the optical gap, $E_c - E_v$. On the other hand, when the correlation energy is negative, only two such optical transitions are possible, and their sum exceeds

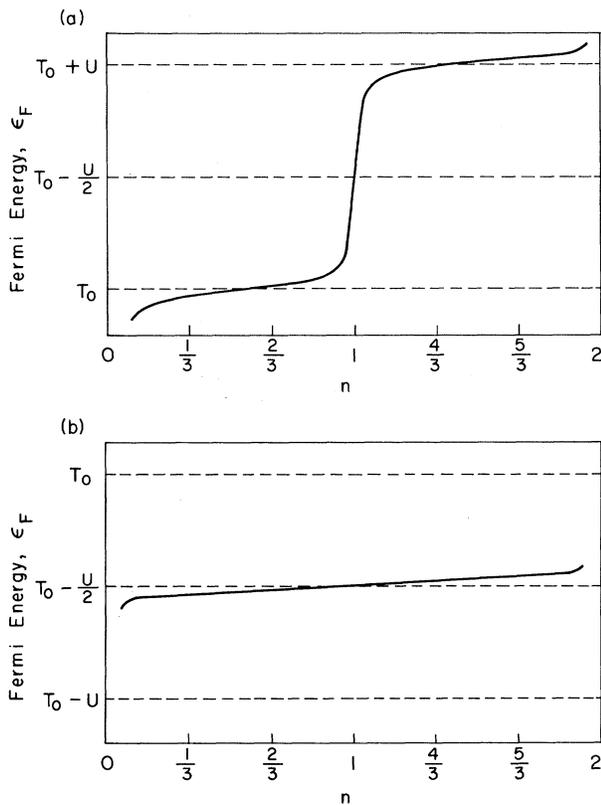


FIG. 1. Fermi energy as a function of electronic density, $n = N/N_0$, at a low but finite temperature: (a) positive correlation energy, U ; (b) negative correlation energy, $-U$.

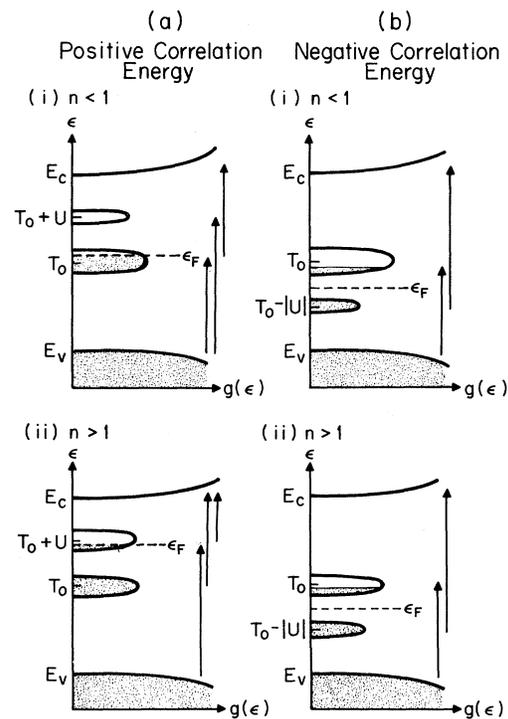


FIG. 2. Density of quasiparticle states for a semiconductor with localized states in the gap relating to a single defect at T_0 : (a) positive correlation energy, U ; (b) negative correlation energy, $-U$. States occupied at $T = 0$ are shaded. Optical transitions connecting localized and band states are indicated by arrows.

the optical gap by the value of U . In principle, this difference could provide an experimental means of distinguishing between the two cases, although the presence of several defect states would preclude such an analysis.

To summarize, the unique features of the results obtained here are (1) that the Fermi energy lies below the energy of the highest-filled quasiparticle states, even at $T = 0$, (2) that this effect leads to an enhanced number of free holes in the valence band and a reduced number of free electrons in the conduction band relative to the values in the absence of correlations, and (3) that the Fermi energy can be pinned as a function of electronic density and temperature, despite the absence of a significant density of states at ϵ_F .

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High-Frequency Conductivity of Electrons in Two-Dimensional Inversion Layers

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The high-frequency conductivity of a two-dimensional electron gas in the presence of ionized impurities is calculated to lowest order in ν_s . The results for the apparent change in mass with frequency and temperature are directly compared with two sets of experimental data and found to be in excellent agreement with the frequency-dependent results.

Electrons accumulated at the semiconductor surface of a metal-oxide-semiconductor interface form an interesting, quasi-two-dimensional, electron gas whose density can be easily varied in the range around $n \sim 10^{12}/\text{cm}^2$. Recent experimental¹⁻⁴ and theoretical investigations^{5,6} of these systems have elucidated many of their simple properties. In the course of these experiments it has become apparent that there is a range of concentrations where the Coulomb interactions among the itinerant electrons play a role in determining the response functions of such systems.

The cyclotron-resonance experiments of at least two groups^{1,2} have shown that the effective mass of the carriers depends on a variety of experimental parameters. In Ref. 1 (hereafter

called I) a systematic variation of mass with frequency and carrier concentration was observed. The work in Ref. 2 focused on variations of the cyclotron frequency with temperature. These workers and others have suggested that such a mass variation arises from the electron-electron interactions. Calculations of the quasi-particle effective mass⁷ lend some credence to these ideas. However it has been clear for some time that these calculations leave out a basic ingredient. Because of the translational symmetry of the homogeneous electron-electron gas and the momentum-conserving nature of the electron interactions, it can be easily shown that the long-wavelength, frequency-dependent conductivity is independent of electron-electron effects.⁸ Impuri-