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BAND STRUCTURE OF POLYACETYLENE, (CH)$_x$

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The one-electron energy bands and densities of states of polyacetylene in both *cis*- and *trans*-conformations have been investigated. The principal issue addressed is whether the itinerant picture alone is sufficient to explain the experimental properties of this material. We conclude that the one-electron model provides an excellent zeroth-order explanation of current observations of optical and transport effects in both pure and doped forms of this unusual polymer.

CARBON CHAIN SYSTEMS of the polyene type have attracted the attention of polymer chemists and physicists for some time. In particular, a fairly large body of spectroscopic data exists for molecular structures ranging from 5–20 CH units in length [1]. These data have engendered much speculation on the physical properties to be expected in infinitely long polyene chains and over the years a number of quantum chemical calculations have been directed to this point [2]. On a theoretical level, the issue has arisen as to whether a single particle picture of itinerant bands can provide a satisfactory description of the electronic structure of the infinite system *vis-à-vis* one requiring electron–electron correlation effects [3, 4]. The recent discovery that polyacetylene, (CH)$_x$, whose *trans*-conformation is the infinite polyene prototype, can be doped [5, 6] to apparently metallic levels with appropriate oxidizing agents has made clarification of this issue paramount. Thus, the applicability of the one-electron concept to (CH)$_x$ in both its pure and doped forms is the major question addressed by this communication.

To help answer this question, one portion of the work presented here involves a novel study of the effect of carbon–carbon bond alternation on the single particle band gap of *trans*-(CH)$_x$. The most important result obtained is that a moderate bond length difference easily produces a gap large enough to agree with the observed adsorption threshold. Another portion entails the calculation of the free electron–hole dynamical effective masses, whose magnitudes are found to agree well with estimates made from plasma edge measurements and with conductivity data on degenerately doped (CH)$_x$. Yet a third part addresses the stability of the metallic state in highly doped (CH)$_x$ by calculating for the first time the band structure of an idealized three-dimensional lattice for *cis*-polyacetylene which reveals amounts of interchain coupling probably

sufficient to suppress Peierls–Froehlich effects. Finally, we show that (CH)$_x$, unlike many other polymeric materials like polyethylene, has bound conduction band states and is, thus, capable of sustaining majority electron conductivity, an assertion which is supported by the recent report of the synthesis of *n*-type polyacetylene [7]. Our principal conclusion is that a single-particle framework can successfully account for all experimental results reported to date on polyacetylene.

For our calculational techniques, we used both the first principles, LCAO, extended tight binding (ETB), method and the semi-empirical extended Hueckel (EXH) method. We will report, herein, primarily the results of the first principles calculation. The ETB method [8] employs a linear combination of Bloch-adapted Gaussian orbitals as its basis set. We used orbitals of double-zeta quality for *s* and *p* states on the carbon atoms. We also examined the effect of adding a single *d* exponent on carbon along with a *p* exponent on hydrogen and found that the filled and low-lying unoccupied bands were virtually unaffected. The crystal potential was constructed from a superposition of atomic potentials which were generated from self-consistent Hartree–Fock charge densities employing the Kohn–Sham–Gaspar local exchange approximation. The starting carbon atomic configuration was sp^3. The potential matrix elements were calculated in mixed direct and momentum spaces to convergence. All overlap integrals of magnitude greater than 10^{-7} were retained. The EXH calculations were done in the usual manner taking into account overlaps up to and including second nearest neighbors.

Figure 1 shows the ETB band structure and density-of-states arising from the 3D crystal structure proposed by Baughman *et al.* [9] for *cis–transoid* polyacetylene. From an orbital analysis of the band eigenvectors, we conclude that the valence and conduction bands in the vicinity of the Fermi energy are due to the π-overlap of
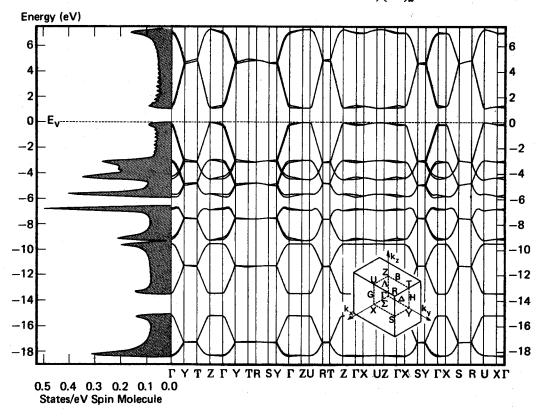
Fig. 1. Band structure and density-of-states for three-dimensional cis-transoid polyacetylene. E_V designates the top of the valence band.

the carbon p-orbitals perpendicular to the chain plane. The sp^2 hybridization of the remaining carbon $2s$, $2p$ orbitals results in bands further from E_F which are formed from the overlap of σ-bonds. In this aspect (CH)$_x$ resembles closely the intraplane bonding in graphite. There are two other features which merit special attention. Firstly, the conduction and valence bandwidths are individually nearly 6 eV along chain directions parallel to k_y and the band gap lies in the near infrared. We calculate the effective mass tensor elements along these directions to be of the order $0.5m_e$ for both holes and electrons. The band gap is found to be approximately 1.2 eV at Z and very slightly larger at Γ. This value agrees well with the experimental determination of 1.17 eV by Bludau et al. [10] for an almost completely cis-polyacetylene film, as do the effective masses obtained from plasma energies in the doped material. It is also in reasonable agreement with the photoconductive threshold energy found by Matsui and Nakamura [11] and recently remeasured by Tani [12]. Thus, the intrachain band properties of polyacetylene remind one of a third or fourth row III—V or II—VI semiconductor or, better yet, two-dimensional graphite.

We note that the space group of cis-(CH)$_x$ is always non-symmorphic, irrespective of differing bond lengths, thus, all bands will be doubly degenerate at at least one

zone boundary. In a single chain, there are always two CH groups (14 electrons) per half-cell translation regardless of bond lengths, so that the Fermi level will invariably lie in the gap between π bonding and antibonding bands. Secondly, the interchain band dispersion near the band gap is never larger than 0.3 eV. In the Baughman structure, neighboring CH chains in the unit cell a-direction have their planes inclined by about 50° to each other, thus, the respective carbon π-orbitals on these neighboring chains are nearly orthogonal and one would indeed expect the very narrow bands seen along k_x (e.g. ΓX) in Fig. 1. We see that the direction of maximum interchain bandwidth is along k_z. This is because in the direct lattice c-direction, the π-orbitals overlap in a slipped geometry similar to that occurring along stacking directions in the conducting TCNQ salts. It is then not surprising that the interchain bandwidth in (CH)$_x$ may closely approximate the intrachain bandwidth in these latter compounds. Although 0.3 eV seems like a small amount, an analysis of the movement of the Fermi level with respect to the top of the valence band yields a value of about 0.2 eV downward for 10% charge transfer from each CH molecule to an acceptor system. This means at this level of doping, a level equivalent to 10 at.% fully charge-transferred AsF$_5$, the Fermi level will still cross bands in the k_x as well as the k_y direction,
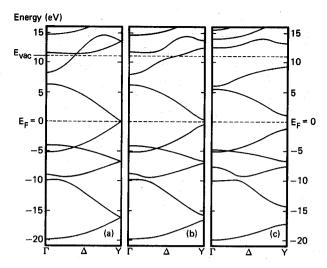
Fig. 2. Band structure of *trans*-(CH)$_x$ for different carbon—carbon bond lengths: (a) uniform (1.39 Å); (b) weakly alternating (C=C: 1.36 Å, C—C: 1.43 Å); and (c) strongly alternating (C=C: 1.34 Å, C—C: 1.54 Å). Note the lifting of the degeneracy at Y as bond alternation occurs.

forming electron—hole pockets along Λ, thus, making particle—particle scattering possible [13] and the resulting Fermi surface will retain a two-dimensional character. Therein may lie the explanation as to why (CH)$_x$ apparently does not Peierls distort at any temperature when degenerately-doped to metallic levels of conductivity.

    The left-hand panel in Fig. 1 gives the total density of states calculated at 208 points in the irreducible part of the Brillouin zone. The area under the curve up to the top of the highest filled valence band corresponds to 2.5 electrons (i.e. the number of electrons of one type of spin on a CH molecule). Our orbital analysis showed the final configuration to be $C(2s^{1.2}\,2p^{3.1})$, $H(1s^{0.7})$ which was nearly the same as our starting configuration. Thus, we do not believe the extension of the calculation to complete self-consistency would materially affect our conclusions.

    In Fig. 2, we compare the results of 1D *trans*-(CH)$_x$ ETB calculations for three different carbon—carbon bond lengths. For the uniform bond length case, shown in Fig. 2(a), the Fermi level passes through the degeneracy point at the zone edge and the system is intrinsically metallic. This was to be expected since the space group for this structure is once more non-symmorphic and all bands have to be doubly degenerate at one zone boundary. Inasmuch as there is only one CH unit (7 electrons) per half-cell translation, the Fermi level will pass through the degeneracy point as it does in 1D polysulfur nitride, (SN)$_x$ [14]. Unfortunately, the details of the crystal structure of both *cis*- and especially *trans*-
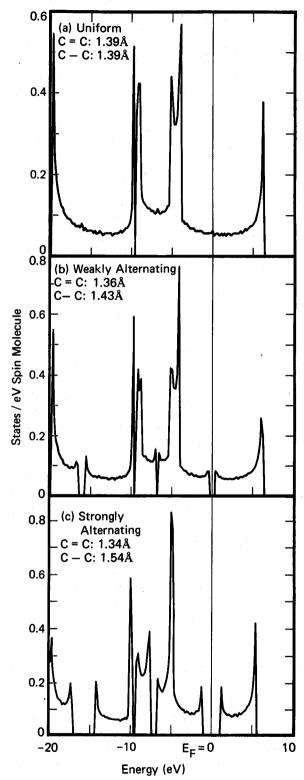

Fig. 3. Densities-of-states of *trans*-(CH)$_x$ for the bond lengths of Fig. 2.

polyacetylene are still not known so the exact carbon—carbon bond lengths cannot be identified. However, the evidence from Raman and IR measurements suggests

some amount of bond alternation is present in both conformations [15]. If bond alternation exists in *trans*-(CH)$_x$, its space group will be symmorphic and a single-particle gap will appear at the Fermi energy. Thus, bond alternation has a far more profound effect on the band structure of *trans*-(CH)$_x$ than for its *cis* counterpart. If interchain band dispersions are similar to those found for the *cis* structure, degenerate doping will again form electron–hole pockets, only now along a zone boundary line as in (SN)$_x$ [16]. The bond lengths used to calculate the structure in Fig. 2(b) were those found to exist near the middle of long carotene molecules [17]. The band gap obtained was 0.8 eV, again in close agreement with optical measurements [10]. The band dispersion widths and effective masses are similar to those found in *cis*-(CH)$_x$. Indeed, we see that from the point of view of choosing which conformation would lead to the highest conductivity on doping, there is little reason to differentiate between the *cis*- and *trans*-isomerizations. On the other hand, bond alternation commensurate with typical single and double bond lengths results in the band structure of Fig. 2(c) with a band gap of 2.3 eV, far in excess of the optical absorption threshold. We can conclude that, when actual crystallographic values are obtained for bond lengths in *trans*-(CH)$_x$, they will probably lie close to those selected for the Fig. 2(b) computation. It is tempting to see bond alternation as a sort of intramolecular Peierls–Froehlich distortion; however, the amount of alternation in *trans*-(CH)$_x$ implied by the optical data, although much smaller than that between typical single and double carbon–carbon bonds, nevertheless seems greater than necessary to lower the ground state energy by just lifting a Fermi degeneracy, even under conditions of commensurability. The likely presence of bond alternation in *cis*-(CH)$_x$, where there would be no metallic state even under uniform bond conditions, suggests that steric interactions may also play a role in producing bond alternation.

For the bands spanning the Fermi level, the ETB and EXH calculations agreed very well for both *cis*- and *trans*-(CH)$_x$ structures. The proportionality of the *trans*-(CH)$_x$ gap to the difference in π-overlap integrals was especially well obeyed. Because ionization potentials enter directly into the EXH method, we were able to establish the vacuum level with respect to the Fermi energy for both *cis*- and *trans*-polyacetylene. The conduction band states in both structures are seen to be bound and the two materials should have negative electron affinities. This is in contrast to other hydrocarbon polymers such as polyethylene, where the conduction band lies above the vacuum level [18]. Thus, polyacetylene, unlike polyethylene, should be capable of sustaining *n*-type conductivity and, in fact,

MacDiarmid and co-workers [7] have succeeded in producing such material by doping with sodium

Figures 1 and 3 contain the densities of states for 3D *cis*-(CH)$_x$ and 1D *trans*-(CH)$_x$, respectively. We note that the density of states near the top of the valence band and bottom of the conduction band is quite small, being around 0.1–0.15 states/eV spin molecule. This value is nearly the same as found at the Fermi energy in (SN)$_x$ [16, 19]. No superconductivity has yet been reported for doped-(CH)$_x$ [6]. From an electronic structure argument, the very low critical temperature found in (SN)$_x$ [20], which has a similar DOS magnitude, argues for an equally weak or absent effect in degenerately-doped (CH)$_x$.

Early spectroscopic studies on polyene chains indicated convergence of the first optical absorption peak toward a finite energy of about 2.25 eV with increasing number of CH units [1]. This observation has been interpreted in two distinct ways: (1) as a single particle gap arising from bond alternation [2] or equation (2) as exciton formation in a Mott–Hubbard system [3]; that is, a system where Coulomb interactions would produce highly localized ground and low-lying excited states. However, it was also observed that the degree of bond alternation decreased with increasing chain length, especially in the middle of the chain, and it was speculated that perhaps in the infinite limit uniform bond distances prevailed throughout the entire chain length [21]. A number of calculational attempts were made to establish whether the Hartree–Fock ground state of the infinitely long uniform polyene chain lies below or above that of an alternating structure [22]. Unfortunately, these efforts produced no definite conclusions. Kertész and co-workers [23] have recently found the alternate structure to be energetically more stable than the regular structure. In fact, the Hartree–Fock solutions for the latter possess charge density wave (CDW) like instabilities. However, the energy gaps they obtained for both the alternating and CDW solutions seem inappropriately large (3–4 eV). In 1974, Ovchinnikov *et al.* [3] (OUK) reviewed the situation and concluded that bond alternation alone could not account for the magnitude of the asymptotic optical gap and it would be necessary to use a Mott–Hubbard model involving Coulomb interaction. In contrast, our calculations show that bond alternation can lead to band gaps as large as 2.3 eV. Because OUK do not state the bond lengths used in their estimate, we are unable to check their alternation gap result with our computational techniques. Moreover, the measured gap in *trans*-(CH)$_x$ ($\sim$ 1 eV) is considerably less than the limiting value inferred by OUK ($\sim$ 2.5 eV). We believe that it is incorrect to extrapolate the position in energy of the absorption peak observed in finite chain segments, where the transition is essentially between the centroids

of molecular orbitals broadened by overlap, to infinite chains in which the transition threshold occurs between band extrema and is influenced both by van Hove singularities in the joint density of states and by a strongly momentum-dependent transition probability. We believe this is why the extrapolated value obtained by OUK and others is so much larger than the experimental number. In addition, we believe OUK misinterpreted the spin susceptibility as arising from exchange interactions between quasi-localized particles where, in fact, it appears the ESR data upon which the interpretation was based are extrinsic in origin [24].

To summarize, we would conclude that the gross electronic properties of both pristine and doped-(CH)$_x$, which have been reported up to now, can be interpreted within the framework of an itinerant one-electron band structure in which Coulomb interactions are negligible. This is not to say that those many-body interactions which give rise to plasmons, Wannier excitons and perhaps even charge density waves, and which can be constructed from single-particle states, will not play an important role in interpreting future experimental results or the finer details of present data.

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Figure 1: The 1979 physical sciences articles most cited in 1979-1980. Authors' affiliations follow each citation. A=1979 citations. B=1980 citations. C=combined 1979-80 citations. D=1981 citations.

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