Concluding Remarks

1 General Conclusions

The charge transfer complexes of macromolecular biomolecules have shown indirect transition across an infrared band gap which is of the order of Peierls gap. An indirect transition involves emission and absorption of a phonon which is furnished by macromolecular flexibility. There are vibrations of bonds of a macromolecule through a lever mechanism. Only CTCs of small molecules show direct band gap. Also there is polaron hopping in some biomolecular solids and their CTCs. Interaction between electron and phonon leads to the formation of a polaron. There is intermolecular hopping of a polaron. This is revealed by a half –power beta density based on Bernoulli trials. If a polaron hops, absorption increases. If it does not hop, absorption decreases. The full-width of half – maximum of envelope (either beta density or Gaussian) shows a linear relation with band gaps found as optical absorption edges. Band gap decreases as FWHM increases. The total change in band gap is only of the order of phonon energy or Urbach tail.

Some organic polyiodide chain complexes have been studied with UV-visible –near IR and FTIR spectroscopy. Indirect transitions are found revealing macromolecular nature of iodine chains. The UV-visible –near IR spectra show that \( A(\lambda) = A_0 \lambda \exp (-b\lambda) \) which is inverse Fourier transform of \( A(k) = b/(b^2 + k^2) \) where \( k \) is wave number. This function has the form of conductivity in Drude model indicating that the polyiodide chain complexes have phometallic nature.

Alternatively, these iodine complexes are ac
photoconductors. The absorption function has also the form of orientational polarizability which arises out of probable presence of orientational Peierls transition.

Spectroscopy of CTCs of amino acids with organic acceptors reveal that these are two-dimensional semiconductors. Layered nature arises out of infinite number of hydrogen bonds induced by charge transfer interaction. Charge transfer interaction of acceptors with hydrocarbon lining of amino acid lead to polarization of amino acids. Thus amino acids with highly polar and positively charged side chains form layered conductors which are CTCs with standard organic acceptors. Amino acid-iodine complexes also reveal two-dimensional nature and show band motion of large polarons as indicated by Gaussian distribution. The amino acids with negatively charged side-chains form CTCs with organic donors. These CTCs show a transition from hopping mechanism of conduction to a band like motion of polarons. A half-part of an envelope is beta density whose other half is a Gaussian distribution. At cut-off wave number, there is transition from hopping across discrete sites to band motion in a continuum. The CTCs of amino acids which are acceptors also reveal a non-linear optical behaviour. The spectra contain 40-50 bands which can be explained with harmonics generated by driving ($w_d$) and pinning ($w_T$) frequencies. The bands are located at $w = n w_d + m w_T$ where $n$ and $m$ are infrared non-linearities.

The CTCs of cytochrome c, hemoglobin and myoglobin with standard organic acceptors show indirect transition across an infrared band gap, in two and three dimensions. These are Hubbard semiconductors with non-universal band gap. TCNQ acts like an enzyme like diphosphoglycerate and TCNQ $^{2-}$ ions
are formed which go into large cavities of myoglobin and hemoglobin. Chloranil complexes show periodic (respective) structures indicating oscillations in the density of states in the infrared spectra. These are square-root singularities along a homomolecular sublattice of segregated stacks of chloranil molecules.

The CTCs of an important biomolecule called biocytin show spin-orbit splitting of valence band except chloranil complex. The valence band is split into three sub bands and there is transition from each of the sub bands to the conduction band. These transitions are found in the infrared spectra. The intraband transitions (transitions among the sub bands) are concluded from these transitions. Biocytin-iodine complex reveals correlated hopping through repetitive structures of beta densities. Hopping becomes a cooperative process and successive hops are induced by the previous hops. Biocytin-chloranil complexe shows again oscillations in the density of states along chloranil stacks.

2 Future Prospects

The solid state spectroscopy of CTCs of biomolecules is just the beginning and a large number of studies can be done on the complexes reported in the present work. The temperature dependence and pressure dependence of electrical resistivity can be carried out to understand conduction mechanism in the CTCs of biomolecules. Such measurements when analyzes according to models of hopping conduction in solid can provide information about dimensionality, at least fractal dimensionality, of the systems. Even if there is any dimensional cross-over at low temperature or at high pressure, it will be marked in such
measurements. Variable range hopping in different dimensions also can be verified. Correlated hopping can lead to oscillations in conductivity and subsequent vanishing of band gap at low temperature and this can be verified. The study of dielectric constant as a function of frequency and temperature also can lead to wide amount of information about the conduction mechanism. AC electrical conductivity can be studied through such measurements. Other physical properties such as thermoelectric power, magnetic susceptibility, photoconductivity, etc. can also throw light on conduction mechanisms and a lot of new physics can be emerge from such measurements.

3 Applications

Most of the CTCs of organic donors and acceptors are semiconductors. Organic CTCs are used in optoelectronic devices. The CTCs of biomolecules also can be used in semiconducting devices such as diodes, transistors, LEDs, photovoltaic devices, photoconducting devices etc. Actually the present study was inspired by models of superconductivity of biomolecules. At present 50 organic superconductors are found at low enough temperatures. High temperature superconductivity is not realized in any organic system. Only a few CTCs become metallic at room temperature and they have chance to become superconducting at low temperature. Exciton mechanism of superconductivity is still not realized in which even a small bandgap semiconductor has chance of becoming superconducting. There were models for DNA, rhodopsin, iodopsin etc. biomolecules for superconductivity but these materials are only semiconductors.
CTC of biomolecules is a new subject and there is enormous scope for studies. If superconductivity is realized in CTCs of biomolecules, there will be a lot of applications whenever superconductors are applied. CTCs of biomolecules can also work as smart materials because of environmental effects, biodegradability and macromolecular flexibility. Physical properties will depend on environmental conditions. Thus this emerging field of CTCs of biomolecules can find applications on a wide scale in physics.
List of Research Paper Publications:

1. Polaron hopping in some molecular solids and their charge transfer complexes by Ashvin Padhiyar and A. T. Oza

2. Spectroscopy of charge transfer complexes of four amino acids as organic two-dimensional conductors by Ashvin Padhiyar and A. T. Oza

3. UV-VISIBLE-IR spectra of some organic polyiodide chain complexes by Ashvin Padhiyar and A. T. Oza