Proposed Research

Research needs to be conducted in parallel in the broad areas of study of the isolated units through the electronic structure of the polymers and interfaces that are involved in real macroscopic formulations. In addition, there is an absence of real understanding of the measured physical properties of the real material including conductivity, magnetism, etc. The development and availability of supercomputers should allow the application of quantum chemistry to larger molecular or oligomeric and chain model units. This should enable a better understanding of the relationship between the molecular and macromolecular architecture, electronic structure, electron-phonon interaction, and charge transport mechanisms. The role of coulomb corrolation has been insufficently explored. Questions arise as to whether it is large or small, and whether it can be controlled to create a ferromagnetic ground state. The effects of interchain interaction and interchain screening need to be investigated. An understanding of photogenerated defects in polymers other than polyacetylene has yet to be developed. The actual conducting polymers synthesized are far from microscopic ordered single crystals. The role of disorder needs to be determined. For example, which properties that are observed are unique to conducting polymers and which are common to all of the disordered systems, for example amorphous silicon. Would doped ordered conducting polymers behave the same or quite differently?

A particularly important question that remains controversial is: why do conducting polymers conduct? Indeed almost all doped polymers have a room temperature conductivity of ten siemens/centimeter. These polymers generally also have a similar concentration of curie spins. Is this central to the properties?

Polymers provide a unique opportunity for the fabrication of new types of composite materials, including the growth of interpenetrating polymer networks as well as growing conducting polymers within microporous systems. These new structures and their properties will challenge the theoretical community to expand the current understanding of composites, for example effective medium theory and Maxwell Garnett theory need be modified to account for these nonspherical structures.