Condensed Matter Theory

Description: There are three major areas of research within the Condensed Matter Theory group:

1 Theory of strongly correlated electron systems aimed at an understanding of charge transport and superconductivity in synthetic metals and low-dimensional magnetism.
2. Theory of x-ray and neutron scattering involving novel instruments at synchrotron and neutron sources.
3. First-principles electronic structure theory directed towards understanding the electronic and magnetic properties of surfaces and bulk systems, with emphasis on the phase stability of metallic alloys.

Program Highlights:

- For correlated electron systems, introduced the idea of charge inhomogeneity in doped Mott insulators, of which the most important current examples are the high temperature superconductors and the manganates. Developed a new mechanism and many-body theory of high temperature superconductivity based on charge inhomogeneity. Showed that charge transport in most synthetic metals cannot be explained by the quasiparticle picture and Boltzmann transport theory.
- In the past few years, there has been a resurgence of interest in low-dimensional magnetism involving, for example, spin chains and spin ladders. Studies of low-dimensional quantum spin models are being used to gain an understanding of the fundamental physics of these materials, and to explain neutron scattering experiments.
- A systematic development of the theory of x-ray and neutron scattering is being undertaken, including a derivation of the expression for resonant scattering in terms of four-time correlation functions, and the use of polarization dependence and analysis to isolate different neutron correlation cross sections.
- A combination of first-principles and model calculations is used to study the bulk and surface properties of materials, with the goals of understanding the underlying physics, interpreting experimental data, and investigating trends. Particular areas of research include the phase stability of multi-component metallic alloys, the study of surface properties in external fields, and the treatment of spin and orbital effects.

Impact:

- The study of "stripes" is now a major areas of research worldwide, with an increasing body of experimental evidence for this unconventional behavior. Charge inhomogeneity, either structural or self-organized, may be responsible for the unusual charge transport in synthetic metals, which pose problems of fundamental interest for condensed matter theory. Oxides in particular are potentially important for applications to electronics in the twenty-first century.
- First-principles calculations allow quantitative predictions of relative phase stability, including the role of defects and microstructure, and can be used to determine basic thermodynamical quantities that may be difficult or impossible to obtain experimentally. The insight obtained and calculations on model systems are the necessary first steps towards the long-promised theoretical "engineering" of new materials.

Interactions:

- There are close ties to experimental groups using techniques such as photoemission, x-ray and neutron scattering' surface tunneling spectroscopy, and infrared spectroscopy, both at BNL and elsewhere.
- There are on the order of 20 active collaborators from institutions throughout the world, including among others, UCLA, LANL, U. Illinois, NIST, U. Conn., Forschungszentrurn-Rilich (Germany), U. Fribourg (Switzerland), and Helsinki Institute of Physics (Finland).

Personnel:

V. J. Emery, M. Blume, R. E. Watson, M. Weinert, S. S. Maslov, V. N. Muthukumar, G. Schneider.

Recognition:

- Twenty-eight invited talks and colloquia/serninars in past two years.
- Two members included in the Institute for Scientific Information's (ISI) list of "1000 Most Cited Physicists, 1981June 1997."

Budget: $750K