MAR06-2005-000333

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

A Revisit to Soliton Theory

XI LIN, MIT

Our recent studies on the soliton theory of conjugated polymers, via Hubbard model and first-principles computations, reveal two subtle points concerning electron-electron correlation and electron-phonon coupling. Significant three-dimensional conformational changes and a sequence of self-localized electronic states are identified and attributed to the presence of soliton. The soliton-induced conformational deformations provide an intrinsic high strain-rate actuation mechanism in optical excitation processes, while the sensitivity of new self-localized states to the presence of local fields provides a high-resolution sensing mechanism for ions and radicals.