Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Quantum transport in Molecular Device[1] PARTHA PRATIM PAL, BRANDON JOHNSON, RANJIT PATI, Michigan Technological University, Houghton, Michigan 49931 — Researchers have taken a lot of interest in designing electronic circuits using molecules ever since the pioneering work of Aviram and Ratner that showed that an organic molecule can be used as a rectifier. Organic molecules with their abundant availability, structural flexibility coupled with their versatile electronic properties are promising candidates for miniaturized electronic devices. To be able to predict the behavior of different organic molecules in an electronic circuit under applied bias, we need to have a detailed knowledge of the electronic structure of the molecule under the influence of the applied electric field. Thus first principles calculations are the best way to get to the root of this problem. In this talk, we report a new approach to model electron transport in single molecular junction, which gives results that match closely with the experimental counterparts. We believe this new approach would give a tremendous boost to the predictive capability of electronic properties of molecular devices.

[1]This work is supported by NSF through grant no. ECCS-0643420.

Ranjit Pati
Michigan Technological University

Date submitted: 14 Nov 2008 Electronic form version 1.4