Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Charge transport in strongly coupled molecular junctions: 'In-phase' and 'out of phase' contribution to electron tunneling[1] PARTHA PRATIM PAL, RANJIT PATI, Michigan Technological University — We report a first principles study on the evolution of charge transport in a two-terminal molecular scale device with the increase in the length of the molecular wire build out of cubane oligomers. In particular, for wires of three different lengths, we look into the relative contribution of the 'in-phase' and the 'out-of-phase' components of the total electronic current under the influence of an external bias. In the low bias regime, the 'out-of-phase' contribution to total current is minimal and 'in-phase' or elastic tunneling of the electrons is responsible for the net electronic current. This is true irrespective of the length of the molecular spacer. In this regime, the I-V characteristics follow Ohm's law and the conductance of the wires is found to decrease exponentially with length which is in agreement with experimental results. However, after a certain 'off-set' voltage, the I-V characteristics become non-linear and the 'out-of-phase' tunneling starts to contribute substantially to the net current.

[1]This work is supported by NSF under grant no. 0643420.

Ranjit Pati
Michigan Technological University

Date submitted: 24 Nov 2010 Electronic form version 1.4