Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Role of dephasing and surface states in Si based molecular electronics[1] HASSAN RAZA, NSF Network for Computational Nanotechnology and School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN — We study the effect of an unpaired dangling bond (DB) on occupied molecular orbital conduction through a styrene molecule bonded to a n++ H:Si(100)-(2×1) surface. For molecules relatively far from the DB, we find good agreement with the reported experiment using a model that accounts for the electrostatic contribution of the DB, provided we include some dephasing due to low energy phonon modes. However, for molecules within 10Å to the DB, we have to include electronic contribution as well along with higher dephasing to explain the transport features. Apart from this, we study the electronic band structure of unpaired and paired DBs, DB wires and clusters on H:Si(100)-(2×1) surface using Extended Hückel Theory (EHT) and report their effect on the Si band gap. An unpaired DB introduces a near-midgap state, whereas a paired DB leads to π and π^* states. The unpaired and paired DB wires introduce states in similar fashion however with larger dispersion. Furthermore, different DB clusters exhibit states that can be interpreted as superposition of states due to unpaired and paired DBs. (cond-mat/0607226,0611417)

[1]This work was supported by the NASA Institute for Nanoelectronics and Computing and ARO-DURINT.

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Date submitted: 20 Nov 2006 Electronic form version 1.4