Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Simulation Studies of Mechanical Properties of Novel Silica Nano-structures KRISHNA MURALIDHARAN, JOAN TORRAS COSTA, SAMUEL B. TRICKEY, University of Florida, QTP NANOROD TEAM — Advances in nanotechnology and the importance of silica as a technological material continue to stimulate computational study of the properties of possible novel silica nanostructures. Thus we have done classical molecular dynamics (MD) and multi-scale quantum mechanical (QM/MD) simulation studies of the mechanical properties of single-wall and multi-wall silica nano-rods of varying dimensions. Such nano-rods have been predicted by Mallik *et al.* to be unusually strong in tensile failure. Here we compare failure mechanisms of such nano-rods under tension, compression, and bending. The concurrent multi-scale QM/MD studies use the general PUPIL system (Torras *et al.*). In this case, PUPIL provides automated interoperation of the MNDO Transfer Hamiltonian QM code (Taylor *et al.*) and a locally written MD code. Embedding of the QM-forces domain is via the scheme of Mallik *et al.* Work supported by NSF ITR award DMR-0325553.

Krishna Muralidharan
University of Florida

Date submitted: 24 Nov 2005 Electronic form version 1.4