Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Effects of the Structure of the Confinement Matrix on Liquid-Liquid Phase Transition and Density Anomaly ELENA STREKALOVA, JIAYUAN LUO, GENE STANLEY, Boston University, GIANCARLO FRANZESE, Universitat de Barcelona, SERGEY BULDYREV, Yeshiva University — We investigate using molecular dynamics the effect of geometrical order in nanoconfinement of liquids with water-like anomalies that display liquid-liquid coexistence at low pressure and low temperature. Our studies using both a ramp and a shoulder interaction potentials show that regularly structured confinement matrices preserve the anomalies, while the phase diagram is shifted to lower temperatures, higher pressures and higher densities with respect to bulk. On the contrary, if the confinement matrices have no geometrical order, we find a drastically different phase diagram: the liquid-liquid coexistence region shrinks significantly and the anomalies are washed out. To understand this effect we calculate the changes in the system at the microscopic level. In the vicinity of the confining nanoparticles we observe that the liquid has a dramatic increase of density that we interpret as an entropic effect. We explain the macroscopic effect of confinement as a consequence of the amount of disorder that is introduced through the configuration of the confining nanoparticles.

Elena Strekalova
Boston University

Date submitted: 10 Nov 2011 Electronic form version 1.4