Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Liquid-liquid transition in supercooled silicon determined by first-principles simulation P. GANESH, Geophysical Laboratory, Carnegie Institution of Washington, M. WIDOM, Department of Physics, Carnegie Mellon University — First principles molecular dynamics simulations reveal a liquid-liquid phase transition in supercooled elemental silicon. Two phases coexist below $T_c \sim$ 1232K. The low density phase is nearly tetra-coordinated, with a pseudogap at the Fermi surface, while the high density phase is more highly coordinated and metallic in nature. The transition is observed through the formation of van der Waals loops in pressure-volume isotherms below T_c.

P. Ganesh
Geophysical Laboratory, Carnegie Institution of Washington

Date submitted: 15 Dec 2008 Electronic form version 1.4