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First-order polymorphic phase transition in supercooled liquid Silicon P. GANESH, Carnegie Institution of Washington, MIKE WIDOM, Carnegie Mellon University — We perform first-principles molecular dynamics simulation of liquid and supercooled liquid Silicon. Looking at the volume dependence of the pressure at different supercooled liquid temperatures, we find a van der-Waals loop, indicating a possible liquid-liquid first-order phase transition. It appears that the transition can be seen only at pressures of about a few GPa. We analyze our data using the zero'th moment of the tetrahedral order parameter, $q_i = 1 - \frac{3}{8}\sum_{j>k}[\cos\theta_{ijk} + \frac{1}{3}]^2$[1], where θ_{ijk} is the angle formed between neighbors 'j' and 'k' and the central atom 'i'. For a perfect tetrahedral arrangement ($\cos\theta_{ijk} = -\frac{1}{3}$) the value of the order-parameter is '1' and for an uncorrelated system its distribution is peaked at '0'. We find that the low temperature liquid has a more tetrahedral open network than the high temperature one, indicating that the transition is between a high-density and a low-density liquid. The electronic density of states along an isochore indicates a sharp drop in metallicity across the transition temperature, which we believe lies around T = 1100K. [1] M. Scott Shell and Pablo G. Debenedetti and Athanassios Z. Panagiotopoulos, Physical Review E **66**, 011201, (2002)

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