Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Diffusion Monte Carlo calculations of Xenon melting under pressure[1] L. SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — The slope of the melting temperature as a function of pressure yields, via the Clausius-Clapeyron equation, important information regarding the changes in density, energy, and entropy. It is therefore crucial to resolve the long-standing differences in melt lines under pressure between Diamond Anvil Cell data (low/flat melt line) and other methods, including density functional theory (DFT) simulations[1] (high/steep melt line). The disagreement for Ta was recently resolved[2] and although a similar situation exists in the literature on Xe,[3] the resolution may be quite different. For example, DFT with its lack of van der Waals forces is a prima facie less credible simulation method for Xe, although excellent agreement has been obtained between calculations of the Hugoniot of Xe and experiments.[4] We investigate whether this theoretical shortcoming is significant for the melting transition by applying diffusion Monte Carlo. The energy differences obtained in this way are compared to the DFT results in order to address any systematic errors that may be present near the melting transition. [1] Taioli et al. PRB **75**, 214103 (2007); [2] Dewaele et al. PRL **104**, 255701 (2010); [3] Belonoshko el al. PRB **74**, 054114 (2006); [4] Root et al. PRL **105**, 085501 (2010)

[1]Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corp. for the US Dep. of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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Date submitted: 07 Dec 2010 Electronic form version 1.4