Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Investigation of the Phase Diagram of Carbon from first principles ALFREDO CORREA, Department of Physics, University of California at Berkeley and Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory, ROGER FALCONE, Department of Physics, University of California at Berkeley, GIULIA GALLI, Lawrence Livermore National Laboratory — The investigation of the phase diagram of carbon has been the subject of experimental research for several decades. Unfortunately progress has been slow due to the extreme temperature and/or pressure required to melt diamond. From the point of view of simulations, it is rather challenging to simulate melting lines under pressure completely from first principles, and only very recently elaborate tools to perform such simulations have been developed [1,2]. We present results for the high pressure portion of the carbon phase diagram, where we have determined new melting lines and predicted metallization pressure and temperature. Our results were obtained using ab-initio molecular dynamics, together with two phase simulation techniques and free energy calculations. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48. [1] S. Bonev et al., Nature 431, 669 (2004) [2] T. Ogitsu et al., Phys. Rev. Lett. 91, 175502 (2003)

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Date submitted: 01 Dec 2004 Electronic form version 1.4