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Melting of Sodium Under Pressure JAN VORBERGER, RONALD E. COHEN, BURKHARD MILITZER, GEOPHYSICAL LABORATORY, CARNEGIE INSTITUTION OF WASHINGTON, WASHINGTON D.C., 20015 COLLABORATION — The bcc, fcc, and liquid phases of sodium are investigated with density functional molecular dynamic (DFT-MD) simulations. We focus on the behavior of the melting curve at high pressure. Diamond anvil cell experiments have determined a melting line with a negative slope at pressures above 33GPa [1]. In the bcc phase, the melting temperature drops from around 1000K to 700K. It decreases even further to 300K in the fcc phase. We have performed simulations for sodium in a range from zero to 100 GPa, temperatures ranging from 300K to 2000K. Equations of State (EOS) for the bcc, fcc and liquid phase are obtained. To investigate the underlying principles of melting in sodium, we study ionic and electronic structure of solid and fluid. Using our EOS, we reproduce positive and negative slopes of the melting line in the proposed pressure regions for the bcc as well as for the fcc phase. [1] E. Gregorianz, O. Degtyarewa, M. Somayazulu, R.J. Hemley, H. Mao, Phys. Rev. Lett. 94, 185502 (2005)

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