The melting of water under pressure

ERIC SCHWEGLER, Lawrence Livermore National Lab, FRANCOIS GYGI, GIULIA GALLI, University of California, Davis — We have investigated the melting of water under high-pressure conditions with a series of first-principles molecular dynamics simulations. In particular, the two-phase approach [1] has been used to determine the melting temperature of water under pressures ranging from 10 to 50 GPa. The effect of molecular dissociation on the structural, dynamical and melting properties of water will be discussed in detail. [1] T. Ogitsu, E. Schwegler, F. Gygi and G. Galli, Phys. Rev. Lett. 91, 175502 (2003)

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