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Phase diagram of silicon using a DFT-based neural network potential OLIVIERO ANDREUSSI, Scuola Normale Superiore di Pisa, Italy & DMSE, Massachusetts Institute of Technology, USA, JOERG BEHLER, Ruhr-Universitaet Bochum, Germany, MICHELE PARRINELLO, ETH Zurich, Switzerland — The phase diagram of silicon is computed by means of Classical Molecular Dynamics. A recently developed [Behler and Parrinello, Phys. Rev. Lett. 98 146401 (2007)] neural-network potential based on Density Functional Theory calculations in the Local Density Approximation is used. This potential was shown to be several orders of magnitude faster than corresponding LDA-DFT calculations, while the accuracy is essentially maintained. Results on the liquid-solid coexistence curve are in good agreement with ab-initio calculations and demonstrate the quality of the neural-network potential.

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