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A Gaussian Approximation Potential for Silicon NOAM BERNSTEIN, U.S. Naval Research Laboratory, ALBERT BARTÓK, Rutherford Appleton Laboratory, JAMES KERMODE, University of Warwick, GÁBOR CSÁNYI, Cambridge University — We present an interatomic potential for silicon using the Gaussian Approximation Potential (GAP) approach, which uses the Gaussian process regression method to approximate the reference potential energy surface as a sum of atomic energies. Each atomic energy is approximated as a function of the local environment around the atom, which is described with the smooth overlap of atomic environments (SOAP) descriptor. The potential is fit to a database of energies, forces, and stresses calculated using density functional theory (DFT) on a wide range of configurations from zero and finite temperature simulations. These include crystalline phases, liquid, amorphous, and low coordination structures, and diamond-structure point defects, dislocations, surfaces, and cracks. We compare the results of the potential to DFT calculations, as well as to previously published models including Stillinger-Weber, Tersoff, modified embedded atom method (MEAM), and ReaxFF. We show that it is very accurate as compared to the DFT reference results for a wide range of properties, including low energy bulk phases, liquid structure, as well as point, line, and plane defects in the diamond structure.

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