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Direct first-principles simulation of shock waves in silicon OLIVER STRICKSON, University of Cambridge, EMILIO ARTACHO, University of Cambridge and CIC NanoGUNE — Density functional theory calculations of thousands of atoms are performed for the direct, non-equilibrium simulation of shock waves, using the SIESTA method and implementation of DFT. We perform a simulation of an elastic shock wave in silicon. We compare simulations using the direct method with equilibrium simulations of post-shock states found such that they lie on the Hugoniot locus, and simulations performed using existing empirical potentials for silicon. System size effects are addressed using conventional empirical interatomic potentials.

Oliver Strickson
University of Cambridge

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