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Quantum-accurate SNAP carbon potential for MD shock simulations JONATHAN WILLMAN, ASHLEY WILLIAMS, KIEN NGUYEN CONG, University of South Florida, MITCHELL WOOD, AIDAN THOMPSON, Sandia National Laboratories, IVAN OLEYNIK, University of South Florida — The ability of molecular dynamics (MD) to realistically simulate the high-strain-rate physics is critically dependent on the availability of high fidelity interatomic potentials capable of capturing the major physics of materials response to high temperatures and pressures. We have developed a Spectral Neighbor Analysis Potential (SNAP) machine-learning potential for high-pressure carbon. SNAP is formulated in terms of the bispectrum components, a set of general four-body geometric invariants that characterize the local neighborhood of each atom. Statistical data analysis is used to train the SNAP potential to reproduce a large set of first-principles training data. In this presentation we describe (1) the generation of the training database comprising the consistent and meaningful set of first-principles DFT calculations; (2) the robust and physically guided fit of the SNAP parameters; and (3) the validation of the SNAP potential in large-scale MD simulations of shock compression of carbon materials.

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