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Molecular dynamics simulation of the shock-induced wurtzite-to-rocksalt transition in CdSe and CdS[1] AIDAN THOMPSON, MARCUS KNUDSON, Sandia National Laboratories — The shock-induced wurtzite-to-rocksalt structural transformation is studied using large-scale molecular dynamics simulation. The primary goal is to understand the atomistic mechanisms underlying the interesting transformation kinetics observed in the case of cadmium sulfide [M. D. Knudson and Y. M. Gupta, J. Appl. Phys, v. 91, p. 9561, 2002]. Since the mechanical and structural properties of cadmium selenide are similar to those of cadmium sulfide, as a first step multi-million atom shock propagation simulations have been carried out in CdSe using the Rabani force field, which has been shown to correctly describe the important bulk phases of CdSe, as well as the wurtzite-to-rocksalt transformation pressure. As a next step a force field for CdS will be developed to enable comparison of similar shock propagation simulations with experiments.

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Aidan Thompson
Sandia National Laboratories

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