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**Optical Properties of LiH From Mixing Rules** DANIEL HORNER, JOEL KRESS, LEE COLLINS, Theoretical Division, Los Alamos National Laboratory — We investigate the use of pressure and density matching mixing rules for predicting the optical properties and equation-of-state (EOS) of lithium hydride for densities from half to twice solid [0.78 g/cc] and temperatures from 0.5 to 3.0 eV. The mixing rules allow us to perform simulations of lithium and hydrogen separately and, from them, calculate properties of the mixture. Using the VASP code, we performed constant  $(N, V, T)$  quantum molecular dynamics simulations for H, Li, and LiH with the results for the mixture (LiH) as a benchmark of the mixing procedures. A finite-temperature density functional theory formulation produces the electronic wave function at each time step within the generalized gradient approximation with projector augmented wave pseudopotentials. Optical properties were determined using the electronic wave function in a Kubo-Greenwood formula. We compare the frequency-dependent absorption coefficient, Rosseland Mean Opacity, and EOS computed via the mixing rules and those from a full LiH simulation.

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