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Ab initio parametrization of bond-polarizability model for Raman spectroscopy of complex Si materials DAVID A. STRUBBE, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Classical inter-atomic potentials can be successful at predicting the vibrations of materials at system sizes intractable by quantum methods. However, to predict Raman spectra, electrons must be re-introduced, for example via a bond-polarizability model which attributes the polarizability to cylindrically symmetrical inter-atomic bonds. Parameters in assumed functional forms are fit to experimental spectra, and then a Raman intensity can be computed for each mode. In the case of amorphous silicon, the existing models do not show satisfactory agreement with experimental spectra. To generate a more accurate and transferable bond-polarizability model, we have instead begun with ab initio calculated Raman tensors for a set of a-Si:H structures [DA Strubbe et al., arXiV:1511.01139]. This atomistic data set allows us to obtain parameters and functional forms for a general model, without confounding errors from the potentials. This Raman model can be used to study large structural models with relevance for photovoltaics, such as medium- and long-range order in a-Si:H, nanocrystalline Si, amorphous/crystalline interfaces, or a-Si:H nanowires, at sizes that would be inaccessible for ab initio calculations. We analyze the applicability of this approach to other materials systems.

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