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A New Charge Model in The Valence Force Field Model for Phonon Calculations¹ CHRISTOPHER BARRETT, University of California, Berkeley, Department of Materials Science & Engineering, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Materials Science Division — The classical ball and spring Valence Force Field model is useful to determine the elastic relaxation of thousand-atom nanosystems. We have also used it to calculate the phonon spectra of nanosystems. However, we found that the conventional point charge model in the Valence Force Field model can cause artificial instability in nanostructures. In this talk, we will present a new charge model which represents the electron cloud feature of the Born charge in a real crystal. More specifically, we have two opposite-signed point charges assigned to each atom, one at its real position, another at a position determined by its neighbor atoms. This innovation allows both electrostatic charges and Born charges to be accurately represented while retaining extreme efficiency. This customized VFF method is developed to be fittable to the results of density functional theory (DFT) calculation. We will present the results of CdSe bulk, surface, and nanowire calculations and compare them with the equivalent ab-initio calculations, for both in their accuracies and their costs.

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Christopher Barrett
University of California, Berkeley,
Department of Materials Science & Engineering

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