TRAJECTORY AVERAGED NORMAL COORDINATE ANALYSIS: POLYMER PARTICLES AND CRYSTALS

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Normal coordinate analysis (NCA) requires the diagonalization of a mass-weighted potential energy second derivative matrix (Hessian matrix). In chemical systems with thousands of atoms, the Hessian matrix can be extremely sensitive to small perturbations in structure, leading to negative eigenvalues (imaginary frequencies) and unstable modes. This problem can be eliminated by performing a molecular dynamics simulation and constructing a trajectory averaged Hessian matrix. With this method, normal coordinates and frequencies have been calculated for polymer particles and crystals with up to 24000 atoms (in contrast to single configuration NCA, which has never succeeded for realistically modeled systems larger than a few thousand atoms). Calculations of heat capacities and other quantities that can be computed from $g(\omega)$ are described in detail for several polymer particles and crystals, as well as recent algorithmic improvements.