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Modeling low frequency vibrational modes of large biomolecules

OTTO SANKEY, ERIC DYKEMAN, Arizona State University — Mechanical oscillations of proteins in their native state are relevant to understanding the flexibility of the protein assembly, the binding of substrates, the mechanical action involved in enzymatic activity, and the vibrational response to light scattering. Often, only the low frequency modes are of interest and coarse grained methods or other approximations are used due to the large size of the dynamical matrix. We introduce a computational approach, which exploits the methodology from electronic structure Order N methods, to find the vibrational modes below some frequency threshold (analogous to a Fermi-level in electronic structure theory). The approach allows systems to be described in atomistic detail. We use a generalized Born force field to model the interactions. Examples of normal modes for icosahedral viruses (e.g. satellite tobacco necrosis virus), tubular viruses (e.g. M13), and enzymes (e.g. lysozyme, HIV-protease, alpha-lytic protease) will be discussed. This effort is motivated by recent experimental work to produce high amplitude vibrations of viruses from impulsive stimulated Raman scattering.

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