Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Low frequency mechanical modes of viruses with atomic detail
ERIC DYKEMAN, OTTO SANKEY, Arizona State University — The low frequency mechanical modes of viruses can provide important insights into the large global motions that a virus may exhibit. Recently it has been proposed that these large global motions may be excited using impulsive stimulated Raman scattering producing permanent damage to the virus. In order to understand the coupling of external probes to the capsid, vibrational modes with atomic detail are essential. The standard approach to find the atomic modes of a molecule with N atoms requires the formation and diagonlization of a $3N \times 3N$ matrix. As viruses have 10^5 or more atoms, the standard approach is difficult. Using ideas from electronic structure theory, we have developed a method to construct the mechanical modes of large molecules such as viruses with atomic detail. Application to viruses such as the cowpea chlorotic mottle virus, satellite tobacco necrosis virus, and M13 bacteriophage show a fairly complicated picture of the mechanical modes.

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Date submitted: 26 Nov 2007 Electronic form version 1.4