Abstract Submitted for the 4CF07 Meeting of The American Physical Society

Calculation of low frequency mechanical modes of viral capsids with atomic detail ERIC DYKEMAN, OTTO SANKEY, Arizona State University — Recently, it has been proposed that impulsive stimulated Raman scattering could be used to resonantly pump large amplitude vibrations into deadly microorganisms such as viruses thereby selectively destroying them. In order to properly calculate the coupling of external probes such as Raman light scattering to vibrational modes of the virus, atomistic detail in the displacement pattern is essential. In this talk I will discuss a new method, based on techniques used in electronic structure theory, to determine the lowest frequency modes (< 20 cm⁻¹) of a viral capsid to atomic resolution.

> Eric Dykeman Arizona State University

Date submitted: 14 Sep 2007

Electronic form version 1.4