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An atomistic approach to viral mechanical oscillations

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Viruses are the simplest "life" form. These parasites reproduce by borrowing the machinery of their host cell. Many are pathogenic to plants, animals, and humans. Viruses possess an outer protein coat (capsid) that protects its genomic material that resides inside. We have developed a theoretical technique to model the very low frequency mechanical modes of the viral capsid with atomic resolution. The method uses empirical force fields and a mathematical framework borrowed from electronic structure theory for finding low energy states. The low frequency modes can be "pinged" with an ultra-short laser pulse and the aim of the light/vibrational coupling is to interfere with the viral life cycle. The theoretical work here is motivated by the recent work of Tsen et al. [2] who have used ultra-short pulsed laser scattering to inactivate viruses. The methodology can be applied to many systems, and the coupled mechanical oscillations of other floppy biomolecules such as a complete ATP binding cassette (ABC transporter) will also be discussed. Co-authors of this work are Dr. Eric Dykeman, Prof. K.-T. Tsen and Daryn Benson.

[1] E.C. Dykeman et al., Phys. Rev. Lett., 100, 028101 (2008).
[2] K-T. Tsen et al., J. of Physics – Cond. Mat. 19, 472201 (2007).