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Modeling virus capsids and their protein binding – the search for weak regions within the HIV capsid OTTO F. SANKEY, DARYN E. BENSON, C. MICHAEL GILBERT, Arizona State University — Viruses remain a threat to the health of humans worldwide with 33 million infected with HIV. Viruses are ubiquitous, infecting animals, plants, and bacteria. Each virus infects in its own unique manner making the problem seem intractable. However, some general physical steps apply to many viruses and the application of basic physical modeling can potentially have great impact. The aim of this theoretical study is to investigate the stability of the HIV viral capsid (protein shell). The structural shell can be compromised by physical probes such as pulsed laser light [1,2]. But, what are the weakest regions of the capsid so that we can begin to understand vulnerabilities of these deadly materials? The atomic structure of HIV capsids is not precisely known and we begin by describing our work to model the capsid structure. We have constructed three representative viral capsids of different CA protein number – HIV-900, HIV-1260 and HIV-1740. The complexity of the assembly requires a course grained model to investigate protein interactions within the capsid which we will describe.
[1] K-T. Tsen, WS.-D. Tsen, O.F. Sankey, J.G. Kiang, Journal of Physics – Condensed Matter, 19 472201 (2007).
[2] E.C. Dykeman, D.Benson, K.-T. Tsen, and O.F. Sankey, Physical Review E 80, 041909 (2009).

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