

Abstract Submitted
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Domain Movement and Dynamics of Norwalk Virus Capsid by Molecular Dynamics (All-Atom and Coarse Grained) Simulations and Normal Mode Analysis¹ MAHENDRA THAPA, JAREK MELLER, MARK RANCE, University of Cincinnati — Norwalk virus is the major cause of epidemic gastroenteritis in humans. The capsid of the virus consists of 180 copies of a single protein which has a protruding (P) domain and a shell (S) domain mechanism of domain movements of the protein is investigated by Gaussian network model(GNM) Dynamics Simulations (MD): Coarse-grained and all-atom (both conventional MD and accelerated MD). Preliminary results are as follows: (i) slow coordinated motions are identified in the hinge regions, (ii) the C-terminus residue interacts with specific residues and (iii) normal mode analysis, coarse grained MD and all-atom simulation generate largely consistent results.

¹University of Cincinnati

Mahendra Thapa
University of Cincinnati

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