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A Molecular Dynamics Investigation of the Physical-Chemical Properties of Calicivirus Capsid Protein Adsorption to Fomites DAVID PEELER, SILVINA MATYSIAK, Fischell Department of Bioengineering, University of Maryland, College Park — Any inanimate object with an exposed surface bears the possibility of hosting a virus and may therefore be labeled a fomite. This research hopes to distinguish which chemical-physical differences in fomite surface and virus capsid protein characteristics cause variations in virus adsorption through an alignment of in silico molecular dynamics simulations with in vitro measurements. The impact of surface chemistry on the adsorption of the human norovirus (HNV)-surrogate calicivirus capsid protein 2MS2 has been simulated for monomer and trimer structures and is reported in terms of protein-self assembled monolayer (SAM) binding free energy. The coarse-grained MARTINI forcefield was used to maximize spatial and temporal resolution while minimizing computational load. Future work will investigate the FCVF5 and SMSVS4 calicivirus trimers and will extend beyond hydrophobic and hydrophilic SAM surface chemistry to charged SAM surfaces in varying ionic concentrations. These results will be confirmed by quartz crystal microbalance experiments conducted by Dr. Wigginton at the University of Michigan. This should provide a novel method for predicting the transferability of viruses that cannot be studied in vitro such as dangerous foodborne and nosocomially-acquired viruses like HNV.

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