# The mechanical properties of the icosahedral shell of Southern Bean Mosaic Virus - A molecular dynamics study - SUPPORTING MATERIAL

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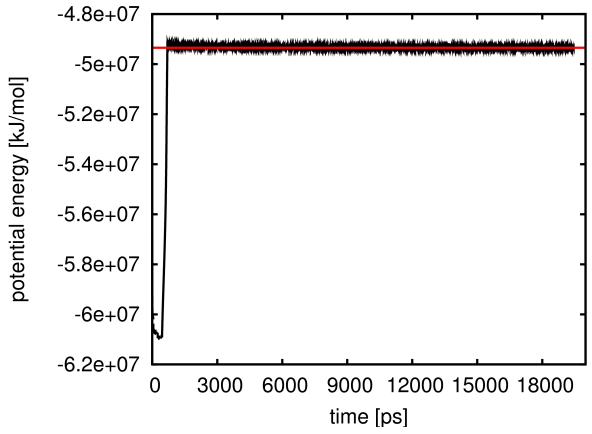


Figure 1: Potential energy of the simulation system during the 19.5 ns equilibration phase. After 3000 ps, the potential energy levelled off at $-4.93 \cdot 10^7$ kJ/mol. This figure was requested by the reviewer.

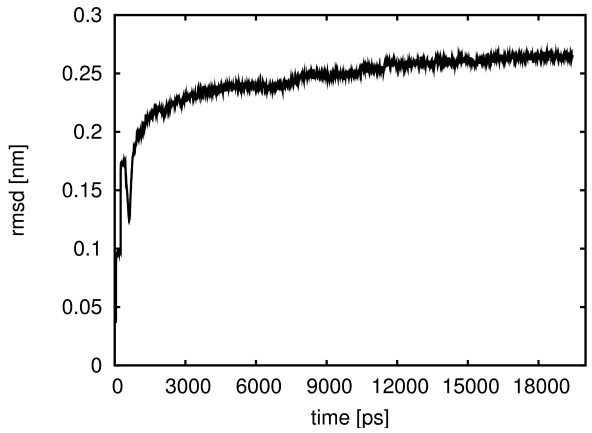


Figure 2: Root mean square deviation (rmsd) of the viral shell heavy atoms with respect to the initial structure after 300 steepest decent steps for the 19.5 ns equilibration phase. After 12 ns, the rmsd remained at 2.62 Å and seams sufficiently converged. The simulation was started with a temperature set to 10 K. Pressure coupling was switched on after 250 ps, resulting in a drop of the simulation box size, which caused a slight compression of the capsid reflected in the rmsd. During heating, the capsid radius relaxed and the protein atoms approached their original positions, causing a dip in the rmsd plot at 450 ps, followed by a slight further expansion.