Text S1. Self Organized Polymer (SOP) model of a virus particle.

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The SOP model of the polypeptide chain was originally designed to address the mechanical properties of proteins (see Refs. [24, 25, 36, 37] the main text). The model has been applied to a variety of biological systems [1–3] and Refs. [15] in main text. In this work, the SOP model has been used to describe each protein subunit forming a virus capsid.

In the topology-based SOP model (Fig. S5), each amino acid residue is represented by a single interaction center described by the C_α-atom, and the protein backbone is represented by a collection of the C_α-C_α covalent bonds with the peptide bond length distance of $a = 3.8$ Å. The potential energy function U_{SOP} specified in terms of the coordinates of the C_α-atoms $\{r_i\} = r_1, r_2, \ldots, r_M$ (M is the total number of residues) is given by:

$$U_{SOP} = U_{FENE} + U_{NB}^{ATT} + U_{NB}^{REP} \tag{S1}$$

In Eq.(S1), the first term is the finite extensible nonlinear elastic (FENE) potential:

$$U_{FENE} = -\sum_{i=1}^{M-1} \frac{kR_0}{2} \log\left(1 - \frac{(r_{i,i+1} - r_{i,i+1}^0)^2}{R_0^2}\right) \tag{S2}$$

where k=14 N/m is the spring constant, and the tolerance in the change of the covalent bond distance is R_0=2 Å. The FENE potential describes the backbone chain connectivity. The distance between the next-neighbor residues i and $i+1$, is $r_{i,i+1}$, and $r_{i,i+1}^0$ is its value in the native structure. To account for the non-covalent (non-bonded) interactions that stabilize the native state, we use the Lennard-Jones potential:

$$U_{NB}^{ATT} = \sum_{i,j=i+3}^{M-3} \varepsilon_h \left[\left(\frac{r_{ij}^0}{r_{ij}}\right)^{12} - 2\left(\frac{r_{ij}^0}{r_{ij}}\right)^{6}\right] \Delta_{ij} \tag{S3}$$

In Eq.(S3), we assume that if the non-covalently linked residues i and j ($|i-j| > 2$) are within the cut-off distance of 8 Å in the native state, then $\Delta_{ij} = 1$; $\Delta_{ij} = 0$ otherwise. The value of ε_h quantifies the strength of the non-bonded interactions. The non-native (non-bonded) interactions are treated as repulsive:

$$U_{NB}^{REP} = \sum_{i,j=i+2}^{M-2} \varepsilon_r \left(\frac{\sigma_r}{r_{ij}}\right)^6 + \sum_{i,j+i+3}^{M-3} \varepsilon_r \left(\frac{\sigma_r}{r_{ij}}\right)^6 (1 - \Delta_{ij}) \tag{S4}$$

In Eq.(S4), a constraint is imposed on the bond angle between the residues i, $i+1$, and $i+2$ by including the repulsive potential with parameters $\varepsilon_l = 1$ kcal/mol and $\sigma_l = 3.8$ Å. These define the strength and the range of the repulsion. In the SOP model, parameter ε_h sets the energy scale. This parameter is estimated based on the results of all-atom MD simulations of the virus particle at equilibrium.

The dynamics of the virus system is obtained by solving numerically the Langevin equations of motion for each particle position r_i in the over-damped limit:

$$\eta \frac{dr_i}{dt} = -\frac{\partial U_i(r_i)}{\partial r_i} + g_i(t) \tag{S5}$$

In Eq.(S5), $U_i(r_i)$ is the total potential energy, which accounts for the biomolecular interactions (U_{SOP}) and interactions of particles with the indenting object — spherical tip (U_{tip}; see Eq.(16) in main text). Also, in Eq.(S5) $g_i(t)$ is the Gaussian distributed zero-average random force, and η is the friction coefficient. To generate the Brownian dynamics, the equations of motion for each C_α-atom are propagated with the time step $\Delta t = 0.08\tau_H$, where $\tau_H = \zeta\varepsilon_h\tau_L/k_BT$ ($\Delta t = 20$ ps for CCMV). Here, $\tau_L = (ma^2/\varepsilon_h)^{1/2} = 3$ ps, $\zeta = 50.0$ is the dimensionless friction constant for an amino acid residue in water ($\eta = \zeta m/\tau_L$), $m \approx 3 \times 10^{22}$ g is the residue mass, and T is the absolute temperature [4, 5]. To perform simulations of nanoindentation of a virus particle, we set T to room temperature and use the bulk water viscosity, which corresponds to the friction coefficient $\eta = 7.0 \times 10^5$ pN ps/nm.

References

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