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Supplementary Information

Quantification and modification of the equilibrium dynamics and mechanics of a virus capsid lattice self-assembled as a protein nanocoating

Alejandro Valbuena and Mauricio G. Mateu

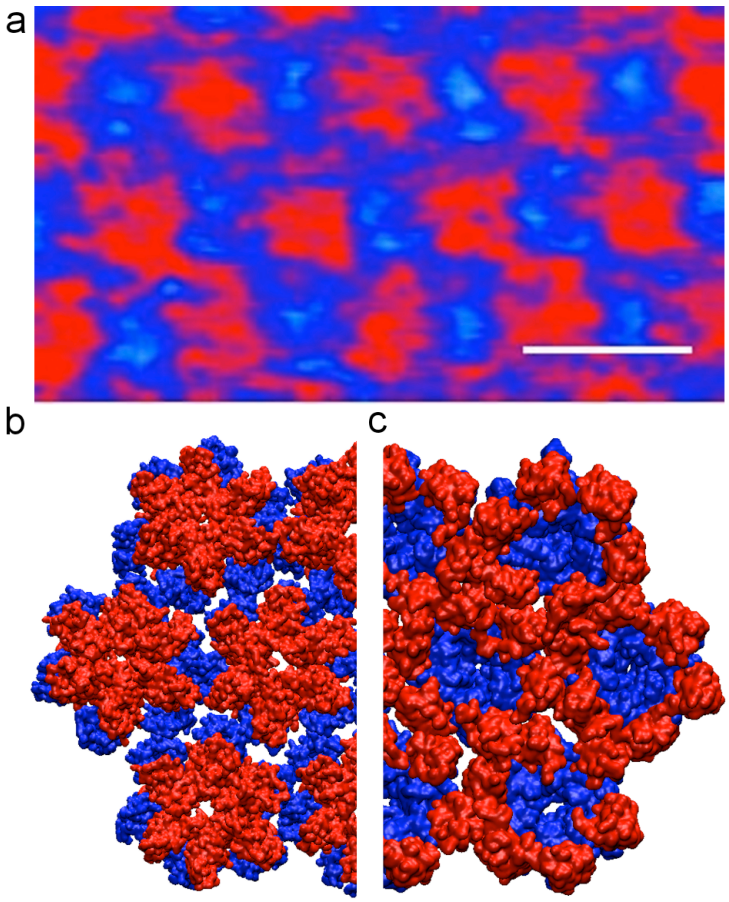


Figure S1. Determining the orientation of the HIV CA lattice on the substrate. (a) High-resolution AFM image of the CA lattice coating the substrate, with height at each point color coded from blue (lower) to red (higher). Scale (white) bar is 10 nm (b, c). Spacefilling model of several hexamers in the HIV CA structure determined by cryo-EM (46), with the CTDs and NTDs respectively colored blue or red, at the same scale shown in panel A. (b) seen from above (NTD on the foreground). (c) seen from below (CTD on the foreground).

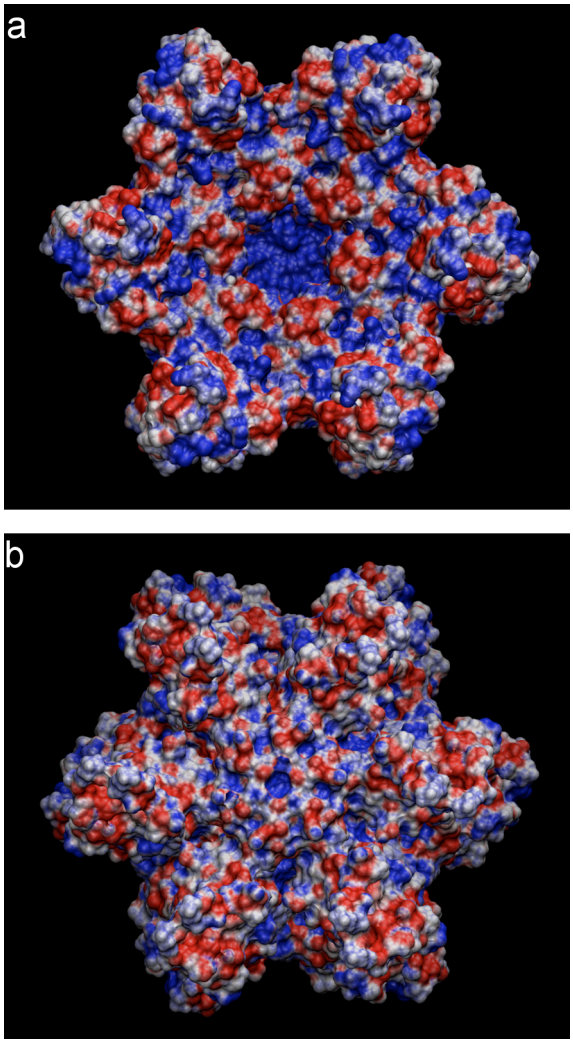


Figure S2. Electrostatic potential distribution in the HIV CA hexamer. a) view from below (CTDs in the foreground) b). View from above (NTDs in the foreground). Electrostatic potential calculation was performed for assembly conditions in solution (pH 8 and ionic strength corresponding to 2.25 M NaCl). Color spectrum from red to blue corresponds to a range between -2 and +2 KT/e.

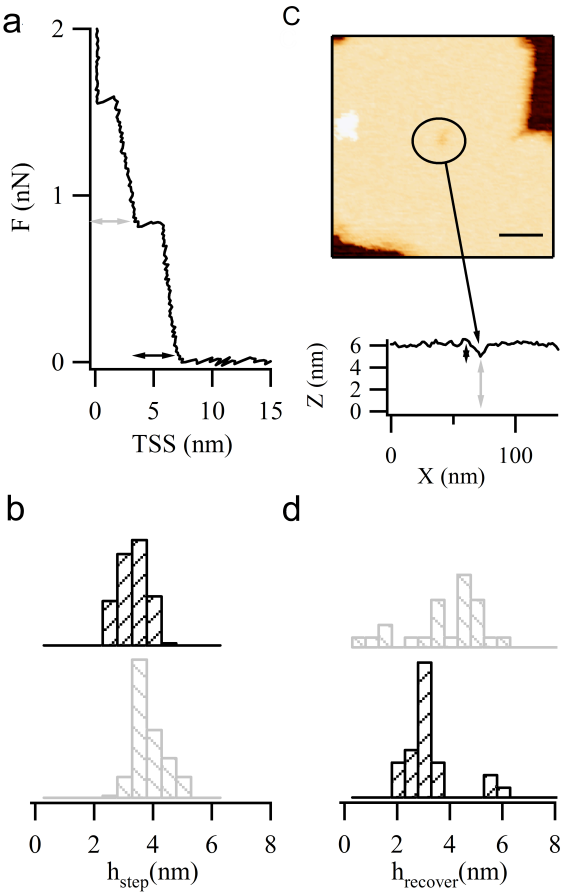
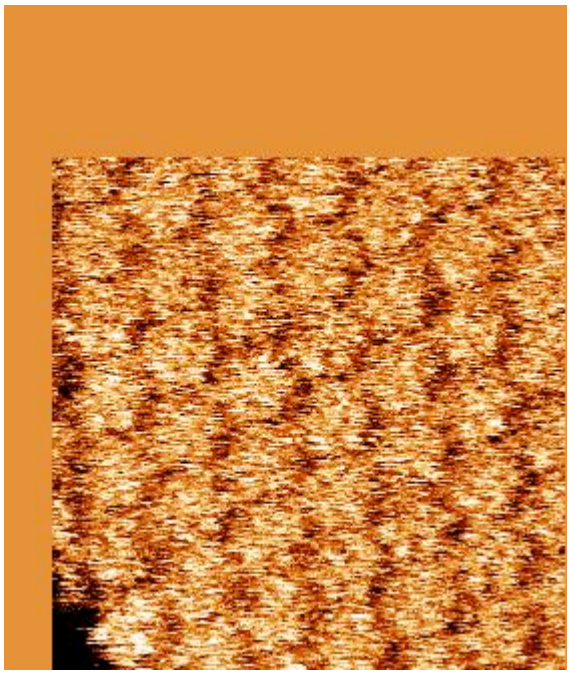
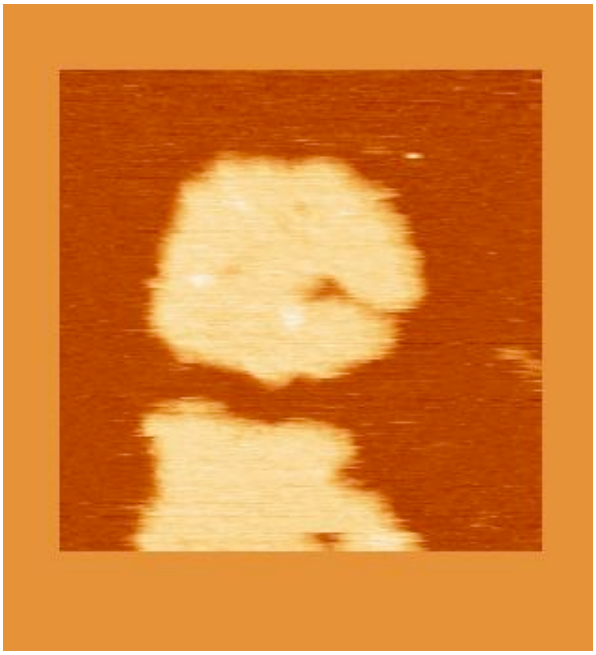


Figure S3. Quantitative characterization of the mechanical disruption of the HIV CA lattice. (a) *A plot of force* versus tip-sample separation for a large indentation of a CA sheet where two force steps (partial disruption events) are observed. The width of the curve from initial contact with the sample, where force starts to increase (at about 6 nm), to the point where the tip contacts the mica substrate and the force increases with an infinite slope (at 0 nm) yields the maximum indentation of the sample (6.2 ± 1.1 nm, N=24), which corresponds to the full height of the CA sheet. The widths indicated by black or grey double arrows correspond to the height of the part of the lattice that is disrupted (or displaced) in the first or second force step, respectively. (b) Distribution of the width of the first (top, black bars) or second (bottom, grey bars) force steps in many curves like that shown in panel A. The corresponding average values for the first and second disruption events were, respectively, 3.0 ± 0.5 nm and 3.5 ± 0.5 nm (N=65). (c) AFM image showing the hole that remains after an indentation (top), and a profile of lattice height and remaining hole depth (bottom). Remaining hole depth was much smaller than maximal indentation, providing evidence of fast self-repair. (d) Distribution of lattice height under the remaining hole (grey double arrow in the profile shown in panel c) and remaining hole depth (black double arrow in the profile shown in panel c; average depth 2.9 ± 1.1 nm, N=24) after many indentations like that shown in panel a.



Video S1. Visualization of slow, large-scale breathing motions in the HIV capsid lattice. See video file. Video total time is 42 min. A depression (darker colours) that appears in the left upper part of the frame reveals a particularly large, transient relative displacement of some neighboring structural elements.



Video S2. Self-repair of the HIV CA lattice after mechanical disruption. See video file. Video total time is 31 min. In the CA patch located in the upper part of the frame, a hole and a fracture were opened by indentation. The fracture was self-repaired first; the hole lasted longer, but was finally self-repaired. In the CA patch located in the lower part of the frame, a fracture was opened close to the border. This fracture caused a reshaping of the patch contour.