Supporting Information

Structural insights into magnetic clusters grown inside virus capsids

M. Jaafar[†‡], A. A. A. Aljabali[¤*], I. Berlanga[¶], R. Mas-Ballesté[¶], P. Saxena[¤,∞], S. Warren[ǀ], G. P. Lomonossoff[¤], D. J. Evans[§] and P. J. de Pablo[†*]

[†] Departamento de Física de la Materia Condensada y Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain
[‡] Instituto de Ciencia de Materiales de Madrid, CSIC, 28049, Madrid, Spain
[¶]Departamento de Química Inórgánica, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[¤] Department of Biological Chemistry, John Innes Centre, Norwich Research Park, Norwich, NR4 7UH, UK
[ǀ] Department of Materials, University of Oxford, Begbroke Science Park, Woodstock Road Oxford OX5 1PF, UK
§ Department of Chemistry, University of Hull, Hull, HU6 7RX, UK
* Present address: Faculty of Pharmacy, Yarmouk University, Irbid, Hashemite Kingdom of Jordan
[∞] Present address: Department of Chemistry, Indiana University, Bloomington, IN 47405, USA
[*] Corresponding author: p.j.depablo@uam.es

1. Co-VLPs on SiO_2

Figure S1 compares both the heights obtained after drying of CPMV virus on HOPG and SiO_2, measured by AFM. Interestingly, a clear effect is observed in the height of the dried CMPV depending on the surface used: the dried Co-VLP are higher when deposited on SiO_2. While eVLPs collapse wall-to-wall on HOPG; when dried in SiO_2 capsids appear, on average, 8 nm higher. A similar case is observed for Co-VLP, which is 6 nm higher on SiO_2 compared with heights observed on HOPG. From these results, we can conclude that the interaction between the wall of the capsid and the surface modulate the process of collapse. Apparently, hydrophobic CPMV-HOPG interactions act as a driving force in the collapsing process. Notably, the CPMV-SiO_2 interaction is much weaker, so it cannot compensate the thermodynamic cost necessary for wall-to-wall collapse. If we compare the results obtained for eVLPs and Co-VLP on SiO_2, a mechanical reinforcement of the virus is observed by the presence of cobalt. In fact, the Co-VLP keeps almost the same height as that observed in solution (23 nm), while on HOPG, a decrease in the height (14 nm) was observed due to increased CPMV-surface interaction. Adsorption results on SiO_2 are less sensitive to the differences between eVLPs and Co-VLP than the results of adsorption on HOPG. Since HOPG elicits a larger collapse it is a better surface than SiO_2 to explore the amount of inner cobalt within the capsid. HOPG shows more restrictive conditions for estimating a top limit of Co inside virus particles.

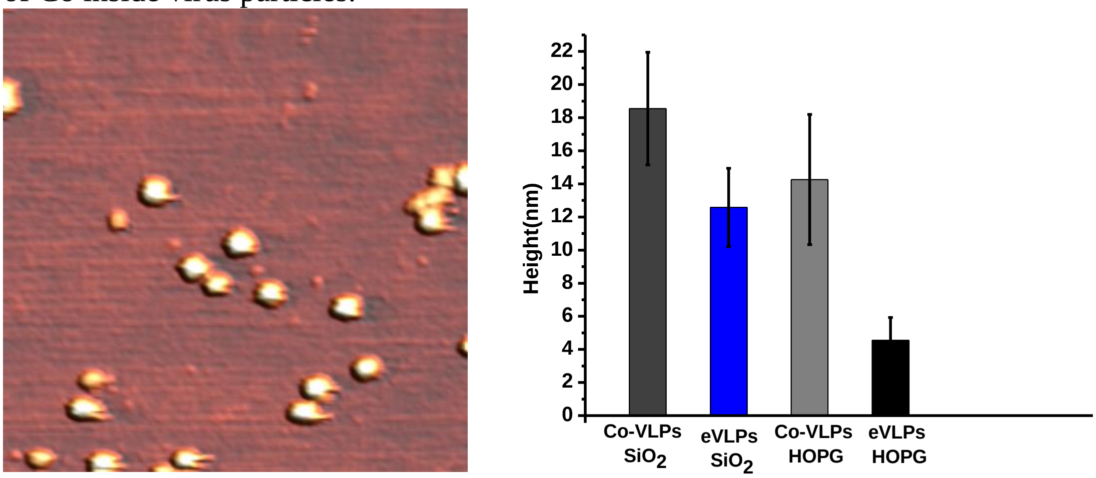

Figure S1: Histograms (right) corresponding to the heights observed by AFM for empty and full particles (left, 1.5x1.5 μm^2) on SiO_2 and HOPG after the drying process.

2 Calculation of Virus Volume and Weight Ratios

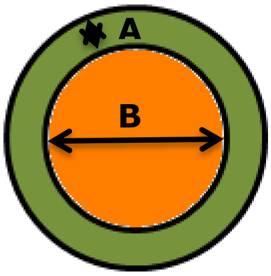

Figure S2

eVLP are protein shells with a total diameter of ~28 nm, and internal cavity diameter of 24 nm, i.e. thickness of the protein shell is 2 nm. With these dimensions and the known density values of the eVLP and cobalt the loading weight ratio of eVLP : Co can be predicted.

Density of cobalt = 8.9 g/cm^3
Density of eVLP = 1.32 g/cm^3

Volume of a sphere = $\frac{4}{3}\pi r^3$

Total Volume of eVLP = A + B = $\frac{4}{3}\pi r^3$ where r = 14 nm

= 11494.0672 nm^3

Volume of inner sphere B = $\frac{4}{3}\pi r^3$ where r = 12 nm

= **7238.2464 nm^3**

Volume of Virus shell coating = Total Volume – Volume of Inner Sphere B

= **4255.8208 nm^3**

If volume is converted into weight:

Co: 1 cm^3 = 1 x 10^{21} nm^3 = 8.9 g
7238.2464 nm^3= x
Weight of Co = **6.442 x 10^{-17} g**

eVLP 1 cm^3 = 1 x 10^{21} nm^3 = 1.32 g
4255.8208 nm^3= x
Weight of eVLP= **0.5518 x 10^{-17} g**

Total Weight = Co + eVLP = 7.0 x 10^{-17}g

For 100% Co loaded eVLP, weight % values should be:

eVLP:	8.7 %	ratio = 0.087
Co :	92 %	

For the TGV data (figure 5)

eVLP:	55%	ratio = 1.2
Co:	45%	

This supports the AFM data that the Co load does not fill the entire virus cavity.

1.2 Dessicated Co-VLPs decrease to 14 nm in height, 9 nm top limit cobalt

If we consider the AFM studies of the dessicated eVLP and Co-VLPs :

Height of flattenened eVLP = 2 nm
Height of Co-VLP = 14 nm where 4 nm corresponds to VLP wall thickness.
Co diameter can be no greater than 5 nm.

1. Assume that the desiccated Co-VLP will have the same VLP content as an eVLP but that it is denser over a smaller area, i.e. density and volume of material has changed but the same weight as calculated above can be expected.

Weight of eVLP= $\mathbf{5.518 \times 10^{-18}}$ **g**

Co volume where r = 2.5 nm	=	523.6 nm^3
Co weight in volume	=	$\mathbf{4.66 \times 10^{-18}}$ **g**
Total weight	=	10.178×10^{-18} g

For this loading weight % values:

eVLP:	54.7%	Ratio 54.7/45.3 = 1.2
Co :	45.3 %	

Similar result to TGV experiments

Considering the mass of solid filling and the AFM/TGV results, the amount of space filled by Co is roughly 0.5 × 100 / 6.4 ~ 10 % of the internal cavity.