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Supporting Information

for

Multiscale modelling of biomolecular corona formation on metallic surfaces

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Supporting material

Contents

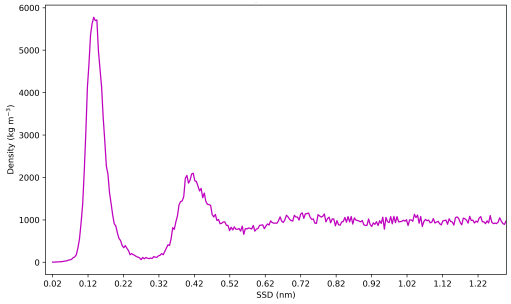
1 Adsorption Free Energies for each SCAs on Al surfaces

Table S 1. Adsorption Free Energies (in k_BT) for Side Chain Analogues (SCA) on the Al(100-110-111) Surfaces from Adaptive Well-Tempered Metadynamics (AWT-MetaD) simulations

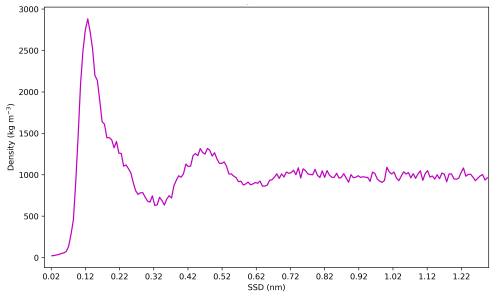
SCA	Class[a]	%[b]	T-group[c]	Charge	E_{min}Al-100	E_{min}Al-110	E_{min}Al-111
ALA	H	7.5	CH_3	0	−2.30	−1.76	−3.33
ARG	C^+	5.2	NH_2	+1	−41.46	−56.26	−55.76
ASP	C^-	5.2	O	−1	−9.34	−20.90	−25.57
ASN	P	4.6	NH_2	0	−19.06	−29.89	−31.52
CYS	P	1.8	CH	0	−5.44	−15.24	−12.77
GAN	P	6.3	COOH	0	−30.58	−30.95	−38.62
GLN	P	4.1	NH_2	0	−25.01	−30.31	−33.93
GLU	C^-	6.3	O	−1	−12.44	−27.08	−23.59
GLY	P	7.1	CH_2	0	−25.91	−37.84	−37.88
HIS	A	2.2	NH	0	−19.88	−37.26	−45.64
HIE	A	2.2	NH	0	−26.15	−32.76	−43.86
ILE	H	5.5	CH_3	0	−2.52	−32.84	−22.78
LEU	H	9.1	CH_3	0	−16.79	−22.59	−5.21
LYS	C^+	5.8	NH_2	+1	−17.64	−30.60	−28.54
MET	H	2.8	NH_2	0	−13.38	−28.72	−24.81
PHE	A	3.9	CH	0	−20.58	−26.02	−42.45
PRO	P	5.1	CH_2	0	−51.68	−50.13	−55.38
SER	P	7.4	OH	0	−6.93	−19.52	−12.65
THR	P	6.0	OH	0	−5.21	−19.51	−12.65
TRP	A	1.3	NH	0	−47.44	−45.23	−63.32
TYR	A	3.3	OH	0	−22.43	−34.29	−56.94
VAL	H	6.5	CH_3	0	−2.83	−17.50	−13.41

[a] H = hydrophobic, P = polar, A = aromatic, and C = charged.,[b]the percentage of AAs composition in proteins ([1]), [c] Terminating group in SCA.

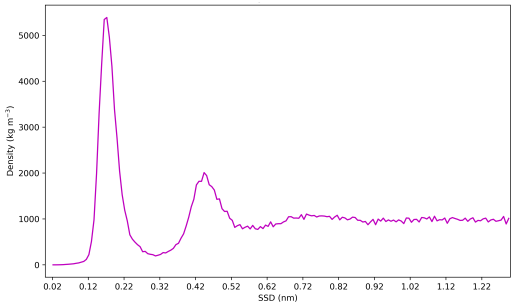
2 Water density profiles for Aluminium slabs



(a) Al-100



(b) Al-110



(c) Al-111

Figure S 1. Water density profile obtained from MD simulation for (a) Al-100, (b) Al-110 and (c) Al-111. The profiles exhibit distinct peaks indicating the presence of water layers near the surface. The first peak, observed at approximately 0.15-0.18 nm, corresponds to the formation of the first water layer adjacent to the aluminum surface. The second peak, occurring around 0.42-0.48 nm, represents the presence of a second water layer.

3 Influence of the NP size on the protein adsorption energies

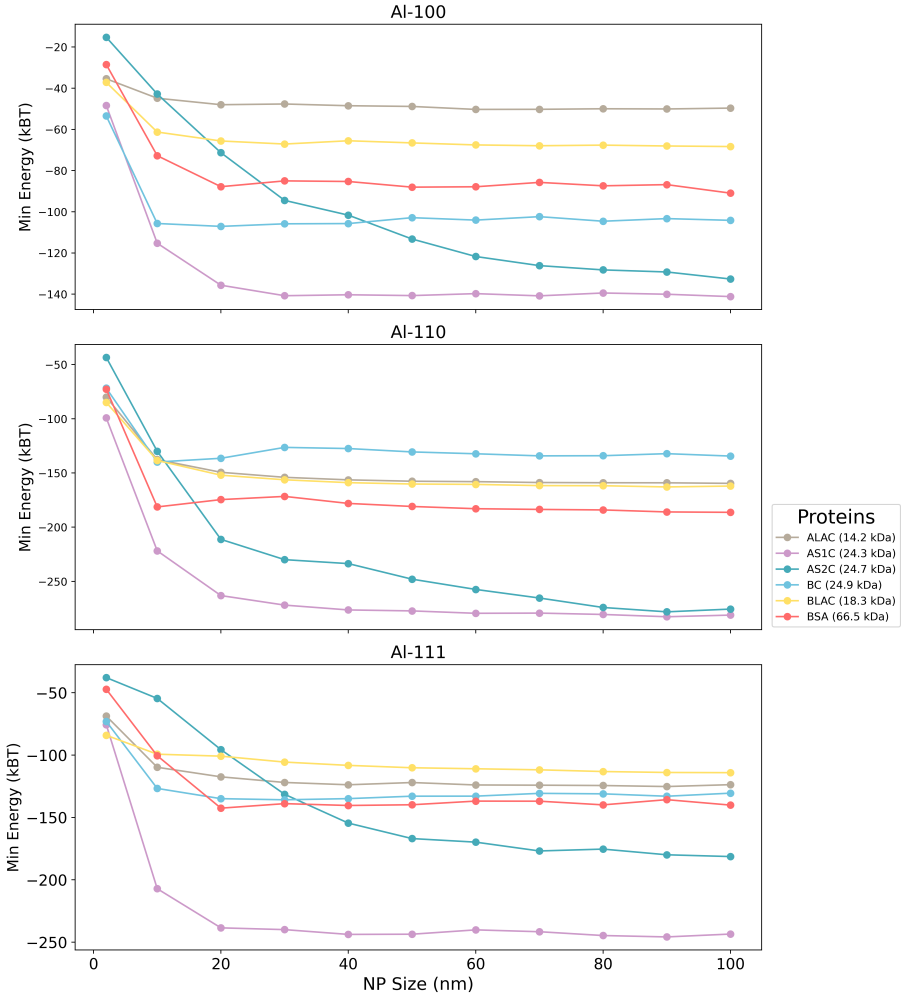


Figure S 2. Energy of adsorption (k_BT) as a function of NP size (R, nm) for six selected milk proteins on Al-100, Al-110, and Al-111 obtained from United Atom model.

4 Milk molecules ranking based on mass abundance in the corona

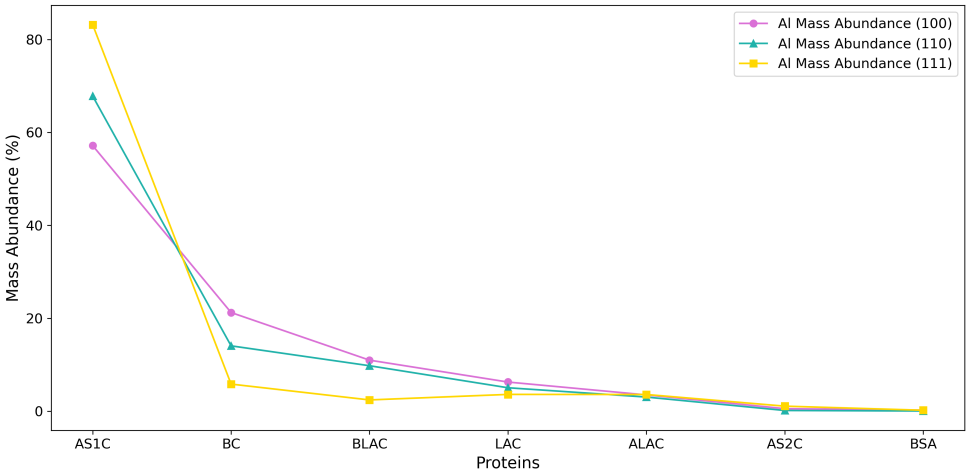
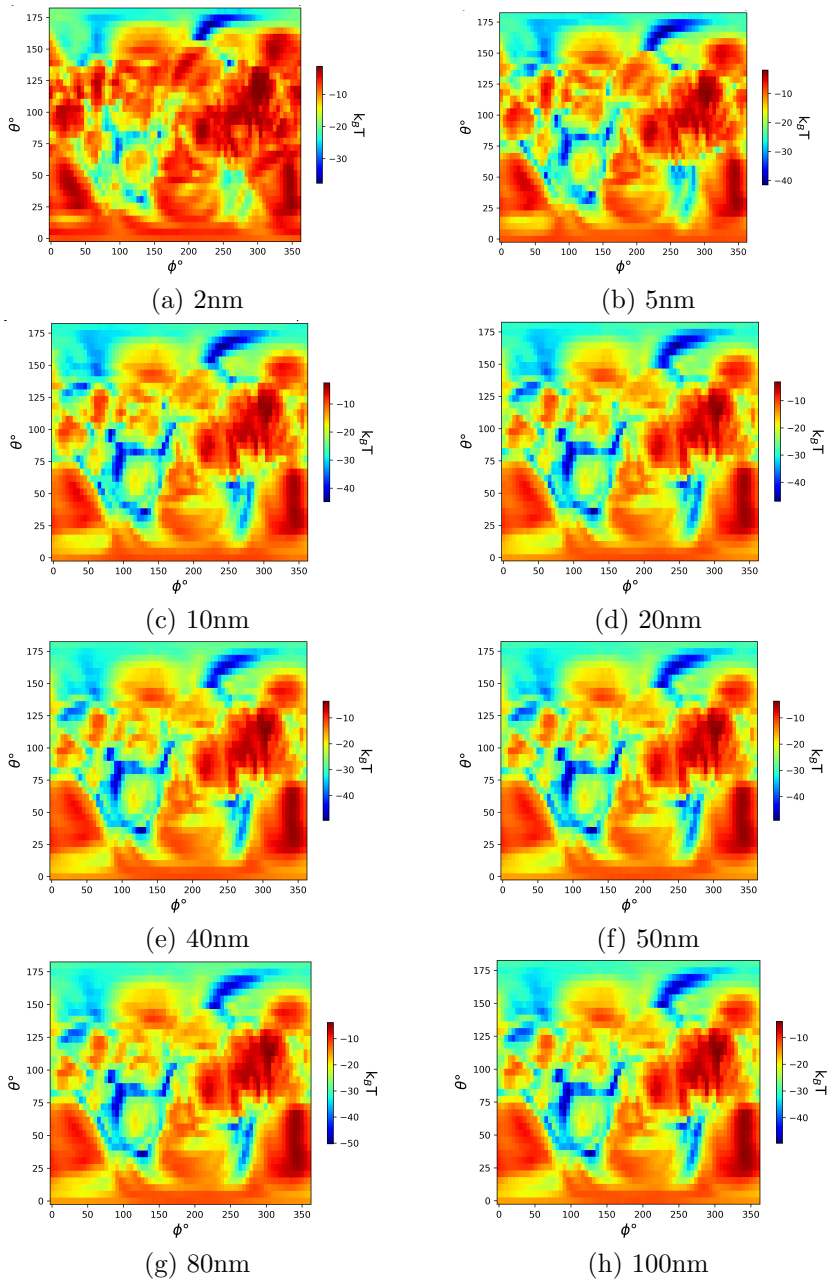


Figure S 3. Protein and lactose mass abundance in the corona on Al surfaces as obtained using the KMC model with molecular displacements, with lactose emerging as the fourth most prevalent compound. The lines are guides to the eye.

5 Example of Al NP size-dependent interaction of α-lactalbumin



(a) 2nm (b) 5nm

(c) 10nm (d) 20nm

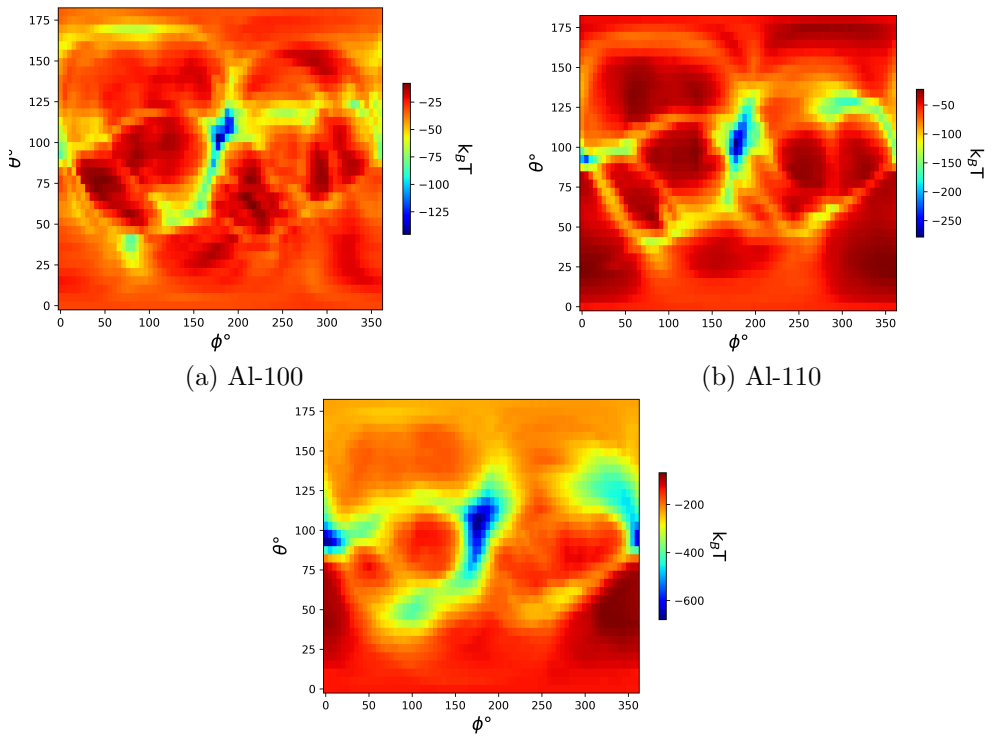
(e) 40nm (f) 50nm

(g) 80nm (h) 100nm

Figure S 4. The heatmap evolution based on Al NP of radius 100 nm for α-lactalbumin obtained from United Atom model.

6 Comparison of interaction of proteins with different Al fcc surfaces

6.1 αs1-casein



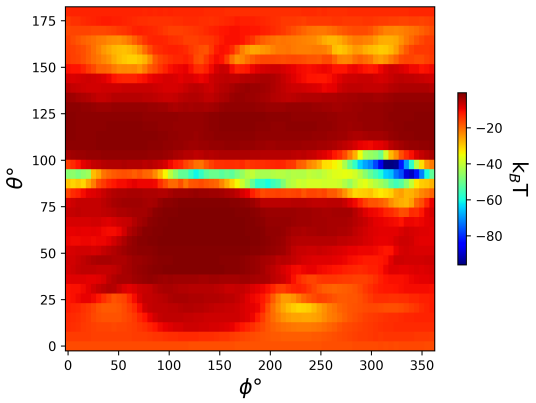
(a) Al-100

(b) Al-110

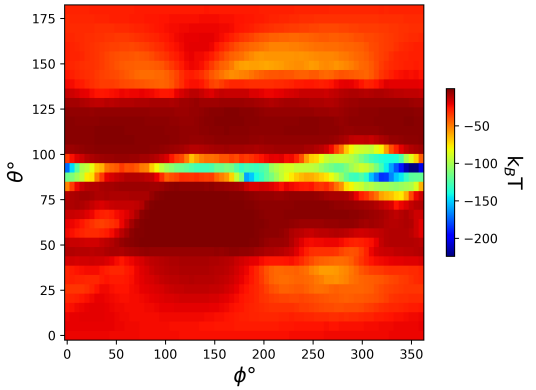
(c) Al-111

Figure S 5. Adsorption energy heatmaps for αs1-casein on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

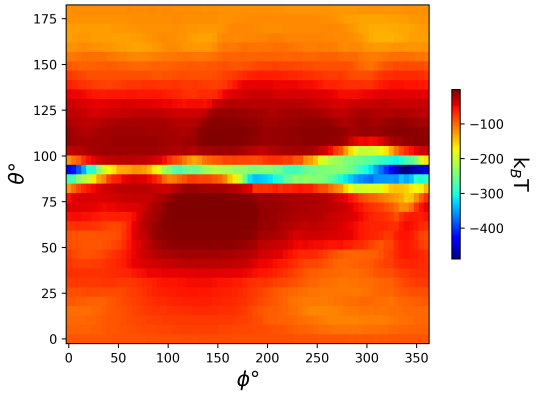
6.2 αs2-casein



(a) Al-100



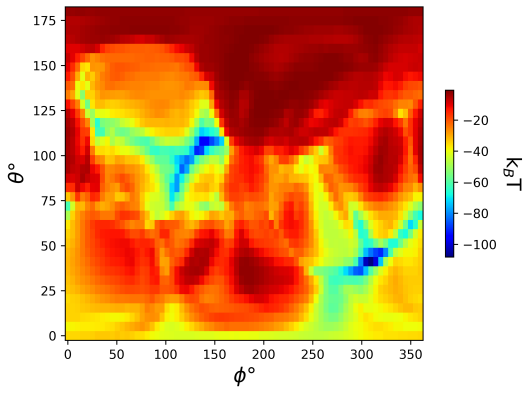
(b) Al-110



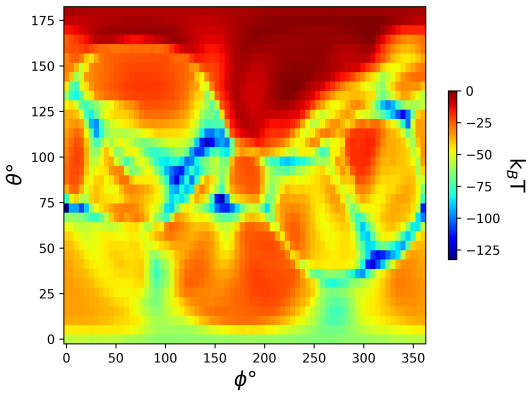
(c) Al-111

Figure S 6. Adsorption energy heatmaps for αs2-casein on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

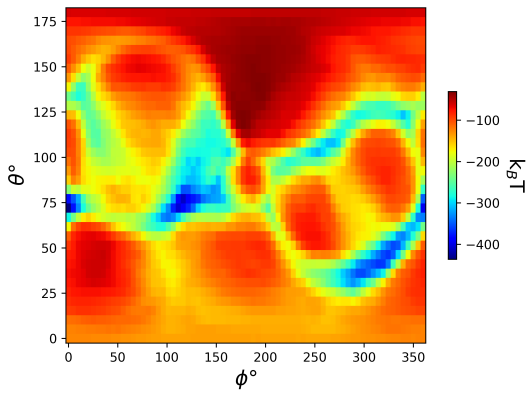
6.3 β- casein



(a) Al-100



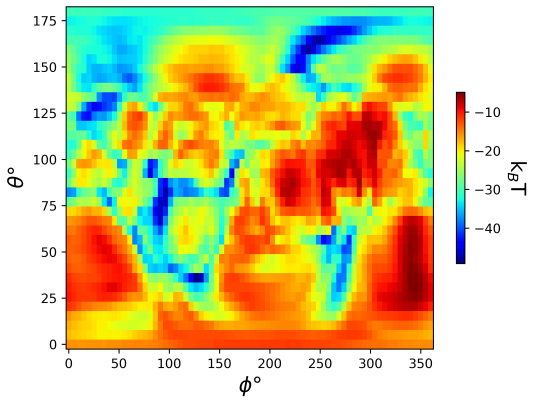
(b) Al-110



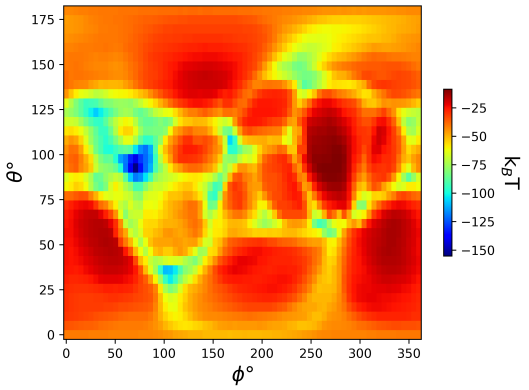
(c) Al-111

Figure S 7. Adsorption energy heatmaps for β-casein on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

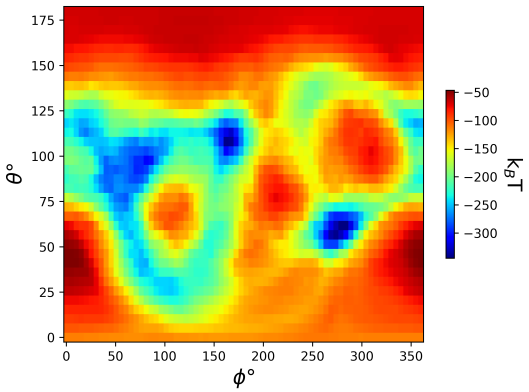
6.4 α-lactalbumin



(a) Al-100



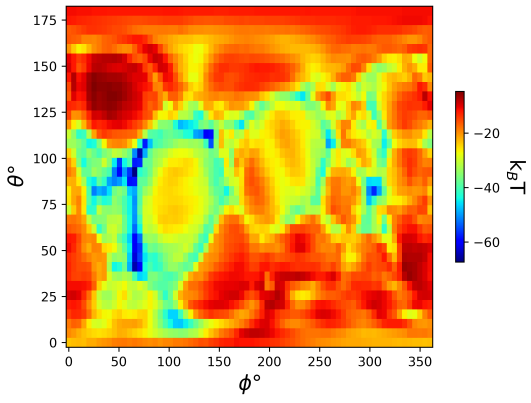
(b) Al-110



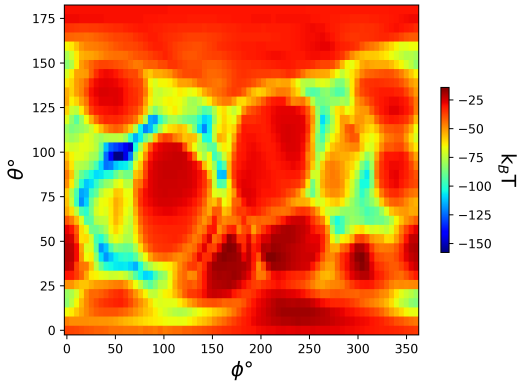
(c) Al-111

Figure S 8. Adsorption energy heatmaps for α-lactalbumin on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

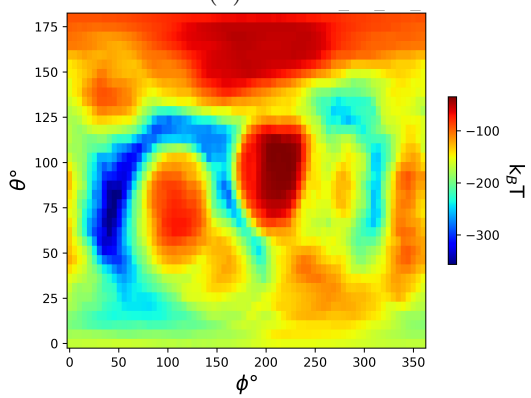
6.5 β-lactoglobulin



(a) Al-100



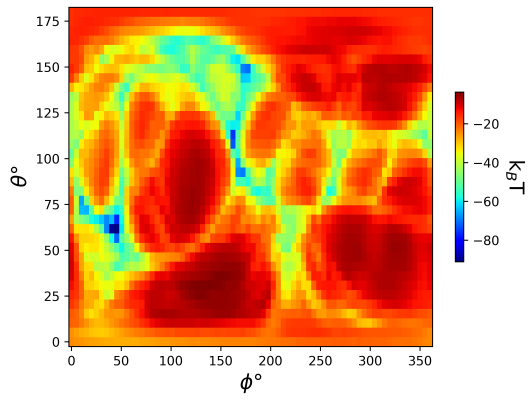
(b) Al-110



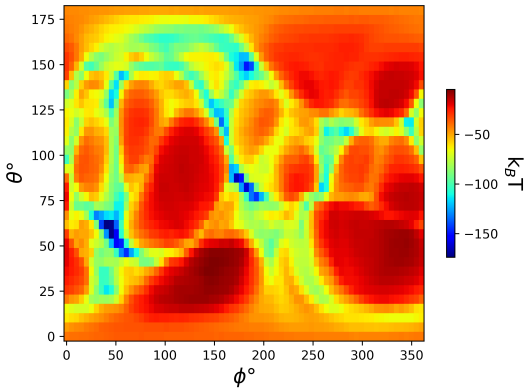
(c) Al-111

Figure S 9. Adsorption energy heatmaps for β-lactoglobulin on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

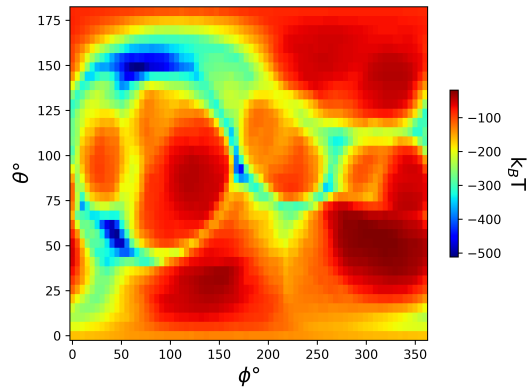
6.6 Bovine Serum Albumin



(a) Al-100



(b) Al-110



(c) Al-111

Figure S 10. Adsorption energy heatmaps for Bovine Serum Albumin on (a) Al-100, (b) Al-110, (c) Al-111 with NP of radius 30 nm obtained from United Atom model

References

[1] Georges Trinquier and Yves-Henri Sanejouand. "Which effective property of amino acids is best preserved by the genetic code?" In: *Protein engineering* 11.3 (1998), pp. 153–169.