Supporting Information

Noncovalent binding phenomena in the adsorption of amino acids on Ag/Au surfaces: A theoretical approach

Catalina Nicolau,[a] Sergi Burguera,[a] María de las Nieves Piña,[a] Antonio Bauzá*[a]

[a]Departament de Química, Universitat de les Illes Balears Ctra. de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain. E–mail: antonio.bauza@uib.es

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Table S1. Values of the density at the bond critical points (ρx100, in a.u.) that characterize the NCIs present in complexes **1–3**, **5**, **6**, **8**, **9**, **11**, **13**, **15–23**, **25–27**, **29**, **31**, **33** and **35–40**. In addition, the values of the laplacian of ρ (∇^2ρx100), the potential (Vx100) and kinetic (Gx100) energy densities as well as the total energy density (Hx100) are also indicated in a.u.

Complex	**ρx100**	**∇^2ρx100**	**Vx100**	**Gx100**	**Hx100**
1	0.54	2.19	–0.47	0.51	0.04
2	0.37	1.67	–0.33	0.37	0.04
3	0.96	3.94	–0.94	0.96	0.02
5	0.49	1.91	–0.41	0.44	0.03
6	1.51	4.09	–0.99	1.01	0.02
8	1.62	4.19	–1.06	1.05	–0.01
9	1.72	7.96	–2.16	2.07	–0.09
11	0.97	1.50	–0.32	0.35	0.03
13	0.98	4.14	–1.02	1.03	0.01
15	1.51	5.77	–1.61	1.52	–0.09
16	0.77	2.52	–0.42	0.53	0.09
17	1.28	4.44	–0.90	1.01	0.11
18	1.71	6.28	–1.42	1.49	0.07
19	1.19	5.43	–1.33	1.35	0.02
20	0.86	1.63	–0.34	0.37	0.03
21	1.26	3.41	–0.69	0.77	0.08
22	0.80	2.56	–0.47	0.55	0.08
23	1.98	5.11	–1.24	1.26	0.02
25	0.95	2.72	–0.55	0.62	0.07
26	2.03	5.36	–1.37	1.36	–0.01
28	1.85	4.61	–1.17	1.16	–0.01
29	1.99	6.97	–1.59	1.67	–0.12
31	1.02	2.25	–0.40	0.48	0.08
33	1.86	4.62	–1.20	1.18	–0.02
35	2.98	6.76	–2.13	1.91	–0.22
36	0.83	2.98	–0.52	0.63	0.09
37	0.89	2.91	–0.53	0.63	0.10
38	1.53	5.46	–1.14	1.25	0.09
39	1.46	5.27	–1.09	1.20	0.11
40	0.93	2.48	–0.50	0.56	0.06

Table S2. Energy Decomposition Analysis into exchange–repulsion ($E_{ex–rep}$), electrostatics (E_{el}), orbital (E_{orb}), electron correlation (E_{cor}) and dispersion (E_{disp}) terms in kcal/mol for complexes **1–3**, **5**, **6**, **8**, **9**, **11**, **13**, **15–23**, **25–27**, **29**, **31**, **33** and **35–40**.

Complex	$E_{ex–rep}$	E_{el}	E_{orb}	E_{cor}	E_{disp}
1	45,1	–11,3	–18,2	–9,9	–8,6
2	8,6	–2,8	–2,4	–3,5	–5,7
3	27,9	0,8	–11,0	–11,4	–13,5
5	30,1	1,8	–13,1	–13,1	–15,1
6	56,6	–13,1	–20,6	–20,1	–21,8
8	76,0	–21,5	–24,8	–25,3	–27,5
9	74,2	–17,1	–29,2	–17,4	–15,1
11	36,0	9,5	–17,9	–16,0	–17,3
13	58,1	–9,7	–22,8	–19,2	–19,0
15	45,2	–5,8	–19,2	–14,9	–15,2
16	27,0	3,4	–13,3	–10,3	–11,6
17	30,8	3,3	–14,4	–11,2	–12,9
18	42,0	–0,5	–18,6	–13,5	–14,9
19	45,3	–3,6	–16,8	–15,7	–17,9
20	26,1	5,1	–14,0	–11,2	–13,0
21	44,2	–10,8	–17,0	–11,2	–10,1
22	11,3	–3,7	–3,1	–4,8	–7,1
23	34,2	–0,8	–12,9	–14,2	–16,9
25	36,2	0,0	–14,9	–15,9	–18,7
26	74,4	–21,2	–26,2	–26,4	–26,7
28	94,9	–30,1	–31,6	–32,1	–33,3
29	77,2	–17,7	–29,2	–20,3	–17,9
31	42,7	6,6	–19,4	–18,8	–21,3
33	71,5	–15,8	–27,6	–23,7	–22,9
35	63,0	–13,9	–25,8	–19,1	–18,4
36	29,4	4,6	–15,8	–11,2	–13,1
37	29,4	4,4	–12,3	–12,2	–15,1
38	42,0	–0,7	–17,4	–15,3	–17,8
39	47,1	–5,5	–16,2	–18,0	–21,4
40	28,1	4,7	–15,0	–12,5	–15,5

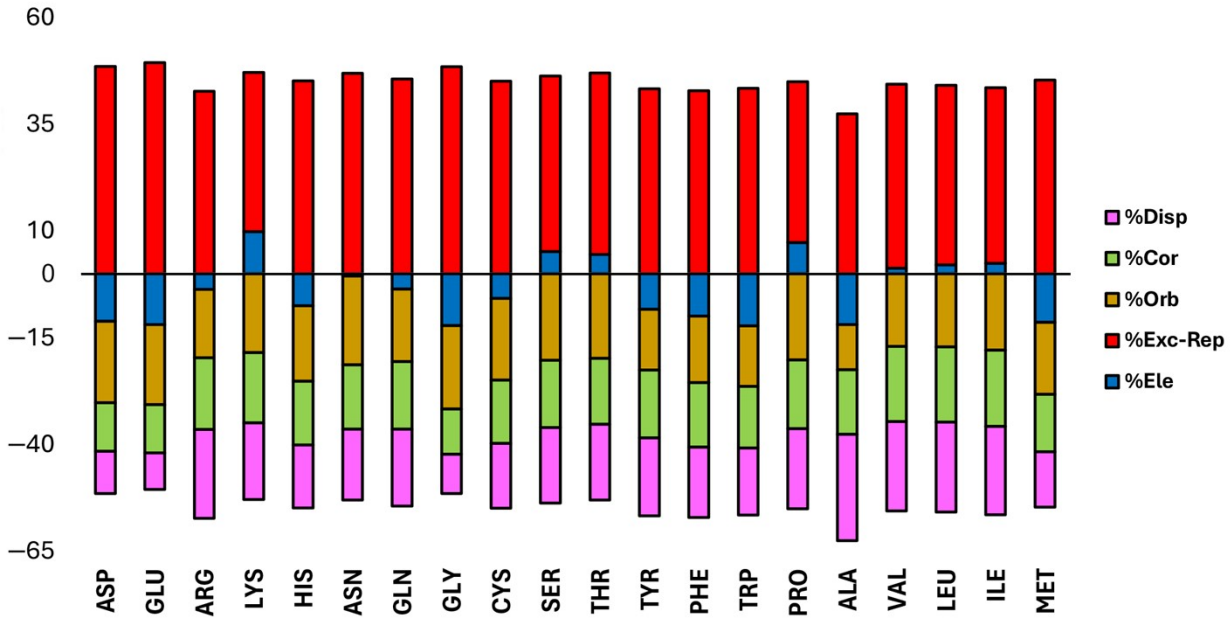

Figure S1. Relative contributions (in %) of the exchange–repulsion ($E_{ex–rep}$ in red), electrostatics (E_{el} in blue), orbital (E_{orb} in orange), electron correlation (E_{cor} in green) and dispersion (E_{disp} in purple) terms to the total interaction energy for Ag26 complexes **1** to **20**.

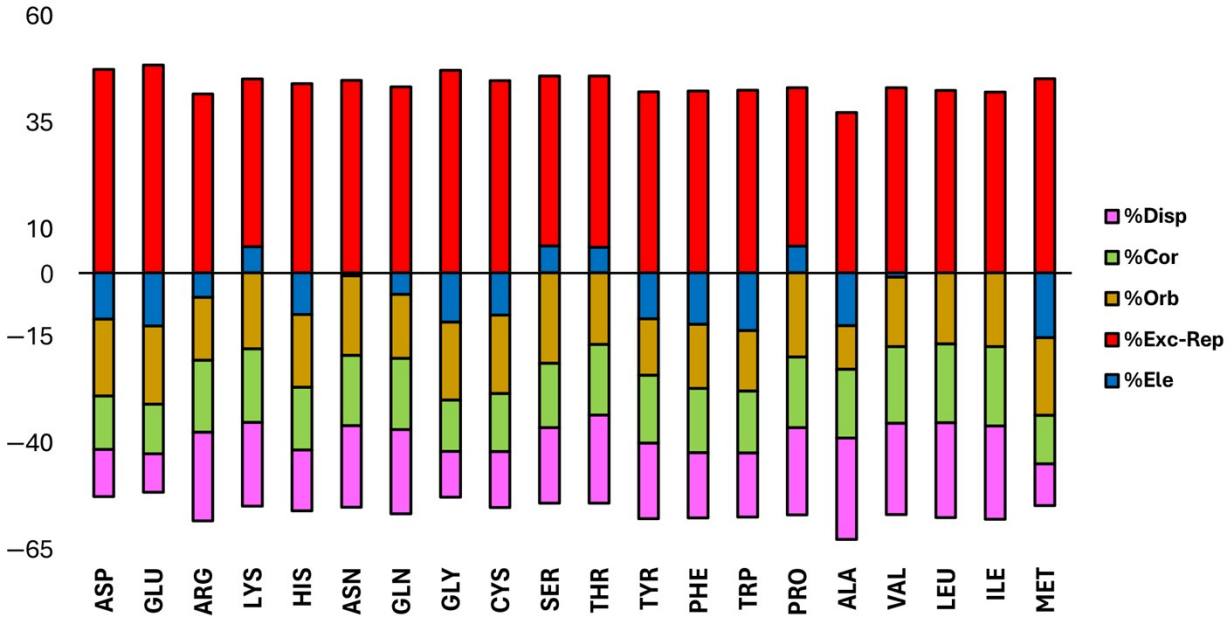

Figure S2. Relative contributions (in %) of the exchange–repulsion ($E_{ex–rep}$ in red), electrostatics (E_{el} in blue), orbital (E_{orb} in orange), electron correlation (E_{cor} in green) and dispersion (E_{disp} in purple) terms to the total interaction energy for Au26 complexes **21** to **40**.