

Supplementary Information

Mechanics of metal-catecholate complexes: The roles of coordination state and metal types

Zhiping Xu

Department of Engineering Mechanics and Center for Nano and Micro Mechanics,
Tsinghua University, Beijing 100084, China.

Email: xuzp@tsinghua.edu.cn

This supplementary information contains:

1. Figures S1.
2. Table T1 and T2.
3. Movies of loaded metal-coordination complexes (for Fe and Ti):
 - M1. Movie of pulling a Fe-based bis-complex
 - M2. Movie of pulling a Ti-based bis-complex
 - M3. Movie of pulling a Fe-based tris-complex
 - M4. Movie of pulling a Ti-based tris-complex

1. Figures and captions

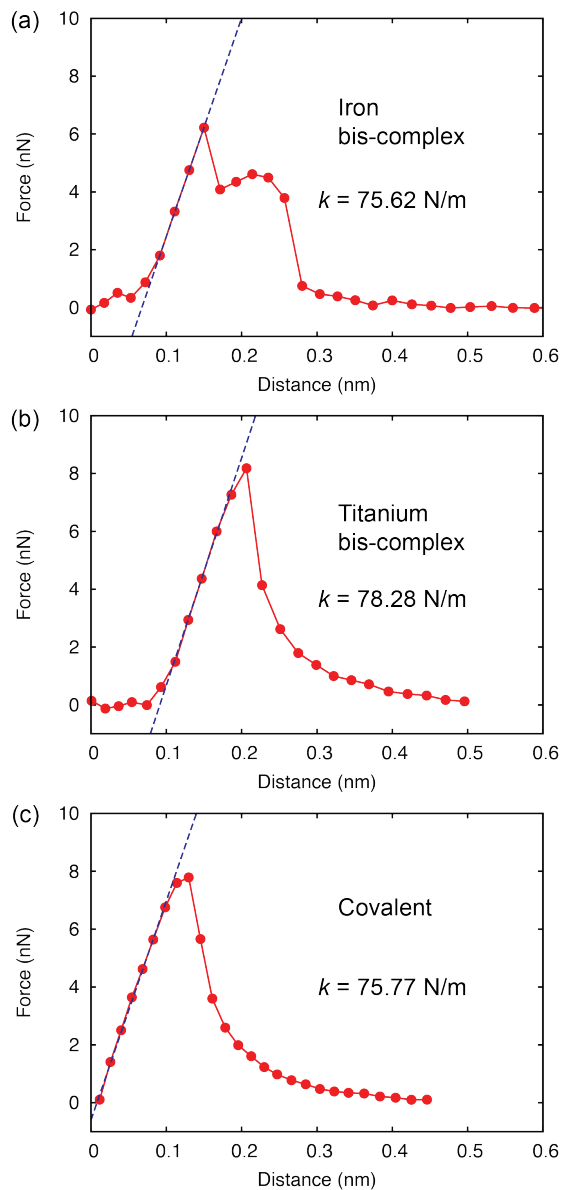


Figure S1 | Stiffness of bis-catecholate-complexes. The stiffness is obtained by fitting (dash lines) to the linear elastic part of force-displacement curve for Fe (a) and Ti (b) respectively.

2. Bond length and angle information for bis- and tris-complexes.

Table T1. Bond length (in unit of Å) and angle information (in unit of degree) for bis-complexes.

	l_1	l_2	l_3	l_4	θ_1	θ_2	θ_3	θ_4
Fe	1.85	1.85	1.85	1.85	85.20	89.88	85.21	89.88
Mn	1.88	1.88	1.88	1.88	85.15	90.52	85.07	90.56
Ti	1.92	1.92	1.92	1.92	82.59	91.47	82.60	91.47
Zn	2.03	2.03	2.03	2.03	83.19	90.47	83.17	90.47
Ca	2.01	2.00	2.01	2.01	79.85	91.66	79.75	91.63
Cu	2.07	2.05	2.01	2.06	81.17	77.45	82.51	77.28

Table T2. Bond length (in unit of Å) and angle information (in unit of degree) for tris-complexes.

	l_1	l_2	l_3	l_4	l_5	l_6
Fe	1.88	1.88	1.88	1.89	1.88	1.89
Mn	1.90	1.90	1.90	1.89	1.90	1.89
Ti	2.00	2.00	2.00	2.00	2.00	2.00
Zn	2.13	2.13	2.13	2.13	2.13	2.13
Ca	2.38	2.38	2.38	2.38	2.38	2.38
Cu	2.05	2.01	2.13	2.11	2.03	2.09

Table T2 (continued)

	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9	θ_{10}	θ_{11}	θ_{12}
Fe	93.58	91.05	84.64	91.05	84.66	90.87	91.07	93.66	91.27	84.68	93.34	91.11
Mn	92.34	91.71	84.16	92.11	84.00	92.23	91.73	92.29	92.55	84.05	91.95	91.68
Ti	97.30	93.12	78.27	92.76	78.20	92.72	92.88	97.34	92.96	78.39	97.46	92.99
Zn	91.88	94.88	79.10	94.76	79.26	94.68	94.88	92.02	94.78	79.23	91.87	94.65
Ca	93.14	99.52	69.65	99.45	69.72	99.21	99.26	93.47	99.44	69.69	93.34	99.31
Cu	93.83	90.96	81.38	94.43	82.29	94.37	93.50	94.60	93.37	79.32	91.31	92.27