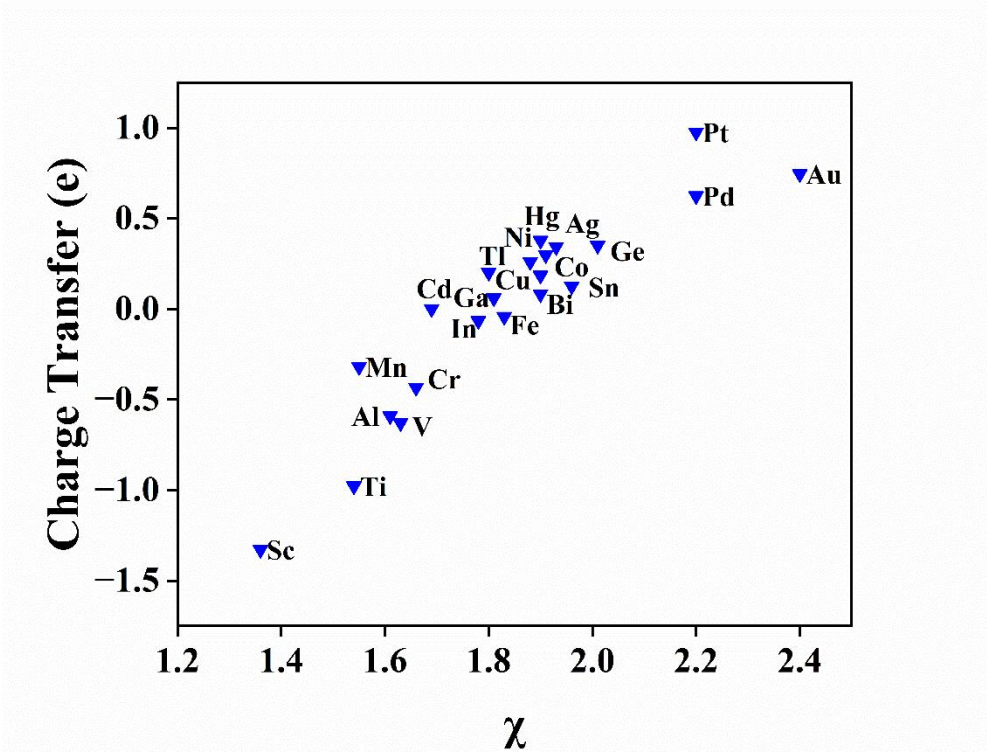
Supplementary Materials

Theoretical design of dendrite-free zinc anode through intrinsic descriptors from symbolic regression

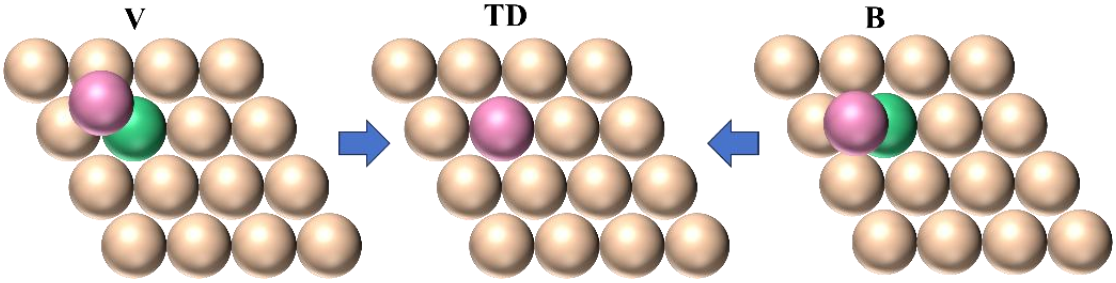
Mengde Kang, Kai Huang*, Jia-hui Li, Honglai Liu, Cheng Lian*

State Key Laboratory of Chemical Engineering, School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, China.

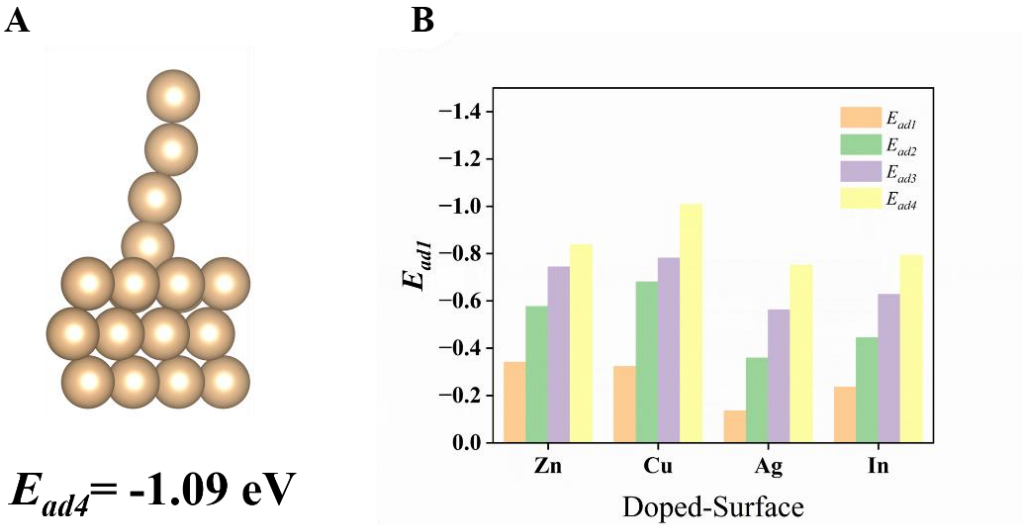
***Correspondence to:** Dr. Kai Huang, Prof. Cheng Lian, State Key Laboratory of Chemical Engineering, School of Chemistry and Molecular Engineering, East China University of Science and Technology, No. 130, Meilong Road, Xuhui District, Shanghai, China. E-mail: hk0537@ecust.edu.cn; liancheng@ecust.edu.cn



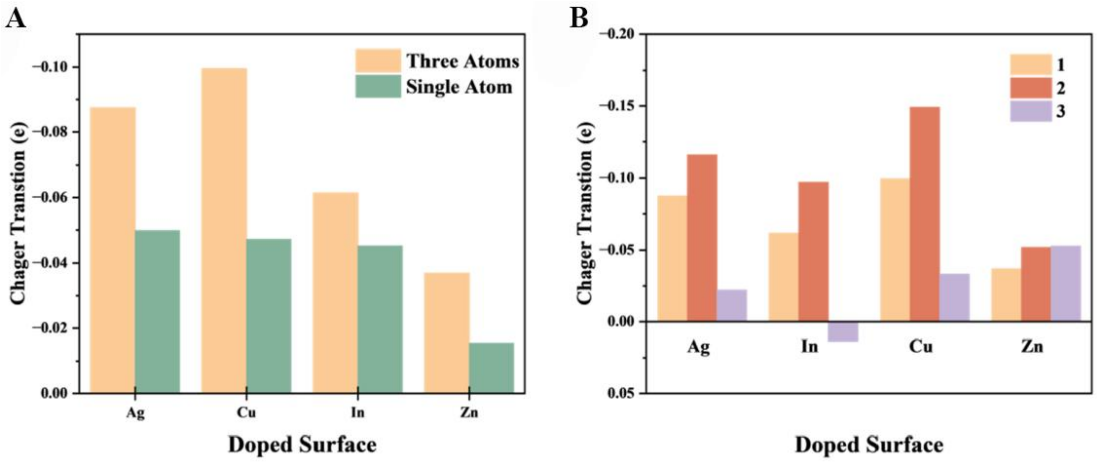
Supplementary Figure 1. The correlation between the electronegativity and the charge transfer of doped atoms.



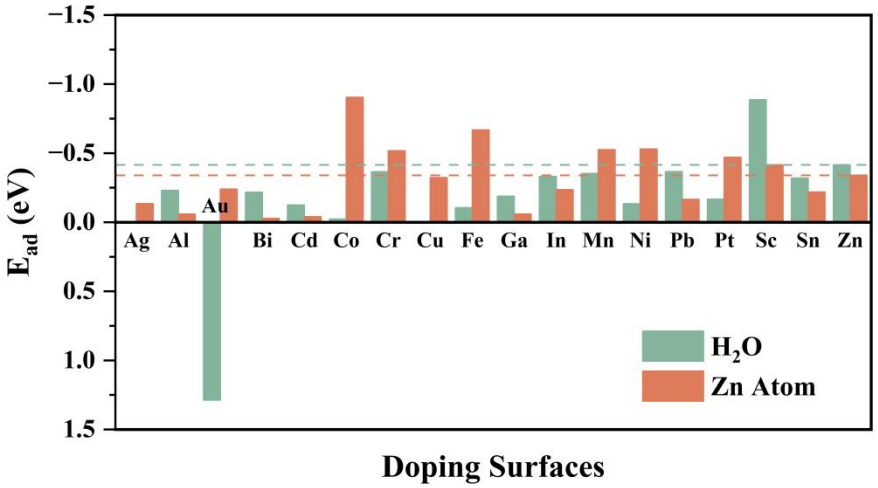
Supplementary Figure 2. The adsorption behavior of one Zn atom on four adsorbed sites. On most of doped surfaces (expect for surfaces doped with Ga, Ge, and Sn), Zn atoms adsorbed on B and V sites will move towards the TD sites, proving that TD sites on these surfaces are the optimal adsorption sites.



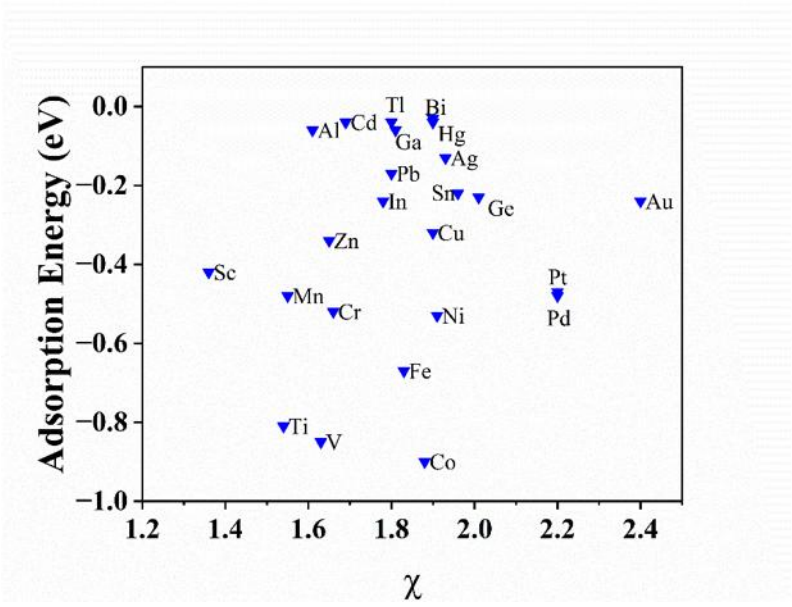
Supplementary Figure 3. (A) The vertical growth trend of zinc nucleus on Zn(002) face; (B) the adsorption energy of vertical adsorption on doped-surfaces.



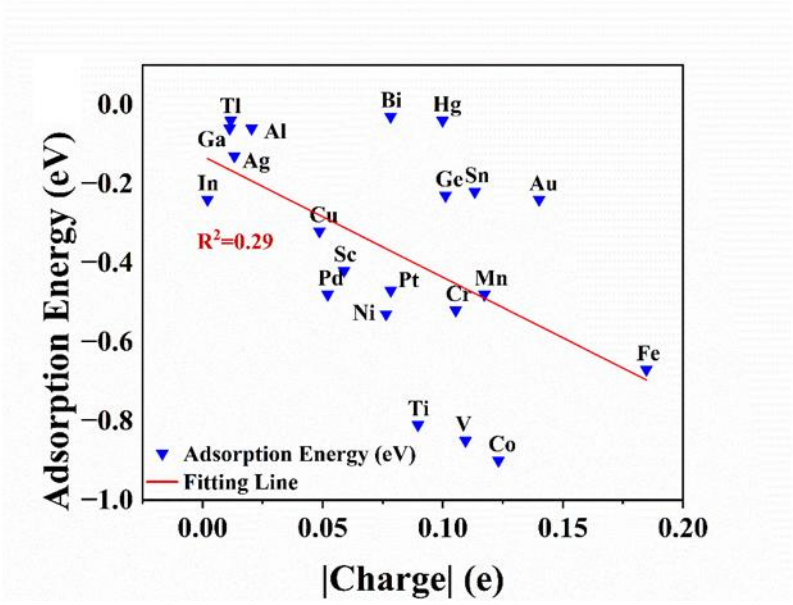
Supplementary Figure 4. The charge transition of the surface absorbed with single Zn atom and three atoms. (A) the firstly adsorbed Zn atom; (B) three adsorbed atoms and the numbers represent the sequence of adsorbed atoms.



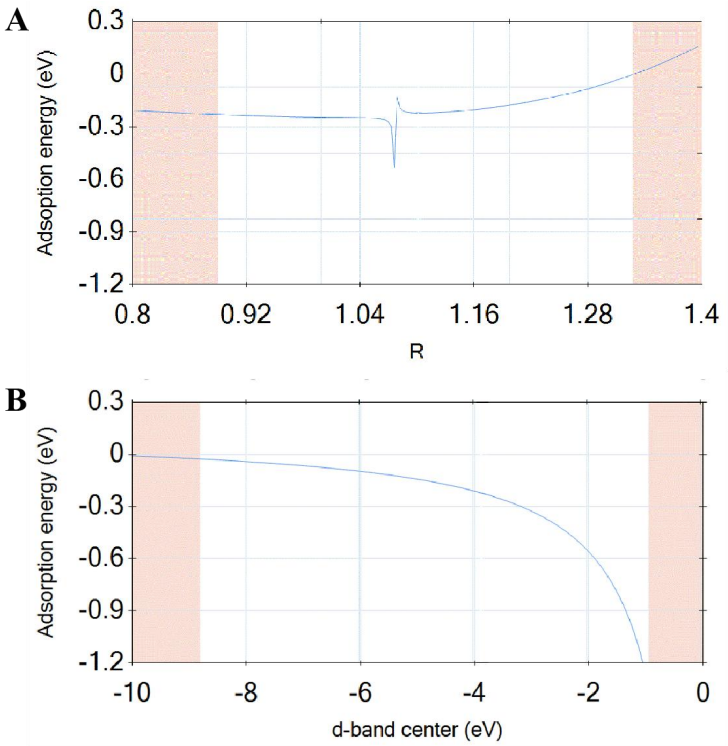
Supplementary Figure 5. The absorption energy of single molecule and single Zn Atom on the doped surface.



Supplementary Figure 6. The relationship between the electronegativity of doping elements and the adsorption energy of single Zn atom on the doping surfaces.



Supplementary Figure 7. The relationship between the absolute value of the charge transfer of doping elements and the adsorption energy of single Zn atom on the doping surfaces.



Supplementary Figure 8. (A) The partial dependence plots of adsorption energy and ratio of radius; (B) the partial dependence plots of adsorption energy and d-band center.

Supplementary Table 1. The formation energy (eV) of doped surfaces and adsorption energy (eV) of different adsorption manners

Doped atom	E_{doped}	u_x	E_f	E_{ab1}	$E_{ab2\text{-}V}$	$E_{ab2\text{-}P}$
Al	-59.27	-3.75	-0.18	-0.06	-0.22	-0.66
Sc	-61.78	-6.33	-0.10	-0.42	-0.24	-1.12
Ti	-62.64	-7.77	0.48	-0.81	-0.35	-1.31
V	-63.23	-8.94	1.05	-0.85	-0.35	-1.36
Cr	-64.07	-9.50	0.77	-0.52	-0.20	-1.08
Mn	-64.01	-9.02	0.35	-0.48	-0.38	-1.07
Fe	-63.09	-8.31	0.56	-0.67	-0.19	-1.29
Co	-62.16	-7.11	0.29	-0.90	-0.46	-1.56
Ni	-61.35	-5.57	-0.44	-0.53	-0.45	-1.22
Cu	-59.32	-3.72	-0.26	-0.32	-0.01	-1.01
Ga	-58.53	-2.91	-0.28	-0.06	-0.29	-0.75
Ge	-59.61	-4.49	0.22	-0.23	-0.26	-0.78
Ag	-58.57	-2.83	-0.40	-0.13	-0.22	-0.73
Cd	-56.59	-0.45	-0.80	-0.04	-0.19	-0.56
In	-58.10	-2.55	-0.21	-0.24	-0.21	-0.77
Sn	-59.21	-3.83	-0.03	-0.22	-0.16	-0.53
Pt	-62.86	-6.06	-1.46	-0.47	-0.52	-1.03
Au	-59.54	-3.27	-0.93	-0.24	-0.26	-0.86
Hg	-55.99	-0.30	-0.35	-0.04	-0.17	-0.55
Tl	-57.60	-2.24	-0.02	-0.04	-0.11	-0.44
Bi	-59.31	-3.87	-0.10	-0.03	-0.16	-0.45
Pb	-58.88	-1.25	-2.29	-0.17	-0.16	-0.60
Zn	-56.61	-1.27	0.00	-0.34	-0.24	-0.96

E_{doped} is the energy of doped-surface; u_x is the chemical potential in bulk phase of doped atom; E_f is the formation energy of doped-surface; E_{ab1} is the adsorption energy of the first adsorbed Zn atom; $E_{ad2\text{-}V}$ is the adsorption energy of the second adsorbed Zn atom adsorbed vertically; $E_{ad2\text{-}P}$ is the adsorption energy of the second adsorbed Zn atom adsorbed parallelly.

Supplementary Table 2. The chemical potential (eV) of doped atoms in bulk phase

Doped Atom	E_{cell} *(eV)*	***n***	u_x *(eV)*
Al	-15.00	4	-3.75
Sc	-12.67	2	-6.34
Ti	-23.32	3	-7.77
V	-17.88	2	-8.94
Cr	-18.99	2	-9.50
Mn	-523.20	58	-9.02
Fe	-16.62	2	-8.31
Co	-14.22	2	-7.11
Ni	-22.28	4	-5.57
Cu	-14.88	4	-3.72
Ga	-23.25	8	-2.91
Ge	-35.94	8	-4.49
Ag	-25.45	9	-2.83
Cd	-3.65	4	-0.91
In	-22.94	9	-2.55
Sn	-30.68	8	-3.84
Pt	-24.23	4	-6.06
Au	-13.09	4	-3.27
Hg	-0.61	2	-0.31
Tl	-20.19	9	-2.24
Bi	-15.47	4	-3.87
Pb	-4.98	4	-1.25
Zn	-2.54	2	-1.27

Supplementary Table 3. The date set of machine learning[1]

Doped atom	*R*	*n*	*I*(KJ/mol)	*A*(KJ/mol)	χ	ε_d(eV)	E_{ad}(eV)
Sc	1.197	3	629.904	18.048	1.36	-2.362	-0.415803
In	1.219	3	555.4944	28.8	1.78	-3.784	-0.235524
Cu	0.934	11	741.7344	118.56	1.9	-2.959	-0.322977
Ag	1.051	11	727.3152	124.992	1.93	-4.785	-0.134702
Pt	1.015	10	860.0448	204.288	2.2	-2.976	-0.469616
Bi	1.328	4	699.408	90.466752	1.9	-3.591	-0.027704
Ti	1.073	4	655.4976	7.584	1.54	-1.651	-0.806733
Fe	0.920	8	758.6304	14.496	1.83	-1.233	-0.668427
Ga	1.117	3	575.9328	41.28	1.81	-4.033	-0.059575
Cd	1.109	12	863.4048	0	1.69	-8.808	-0.043195
Au	1.051	11	885.648	221.62848	2.4	-4.494	-0.239012
Pb	1.277	5	712.0032	34.944	1.8	-3.423	-0.165125
V	0.985	5	647.6352	50.4	1.63	-1.102	-0.854681
Co	0.912	9	756.576	63.552	1.88	-0.946	-0.904391
Ge	0.890	4	758.3424	118.34035	2.01	-3.666	-0.228384
Mn	1	7	713.664	-50	1.55	-1.448	-0.483827
Hg	1.131	12	1002	0	1.9	-4.494	-0.037000
Tl	1.248	3	586.3872	36.192	1.8	-7.211	-0.040796
Cr	0.942	6	649.584	63.936	1.66	-1.475	-0.517165
Ni	0.9124	10	733.4304	110.976	1.91	-1.472	-0.525084
Pd	1	10	800.3424	53.952	2.2	-2.74	-0.477816
Sn	1.153	4	705.0144	106.75843	1.96	-3.884	-0.218760

R is the ratio of the radius of doped atoms to that of Zn atom; *n* is the number of valence electrons; *I* is the first ionization energy of the doped elements; *A* is the first affinity energy of the doped elements; χ is the electronegativity; ε_d is the d-band center of doped surface; and E_{ad} is the adsorption energy of single Zn atom on the doped-surface.

Supplementary Table 4. The formula for calculating adsorption energy obtained by symbolic regression method

The formula obtained after regression:

$$E_{ad1} = \left(\left(c_1 \cdot R + ((c_1 \cdot R)^3 + \frac{\left((c_2 A)^{1/3} + c_3\right)}{c_4 \cdot \varepsilon_d}\right) \cdot \left(c_5 \cdot \chi + \frac{(c_1 \cdot \varepsilon_d)^{1/3} \cdot c_7}{(c_3 \cdot R)^3 \cdot c_9 + c_{10}} + c_{11}\right)\right) \cdot (c_{12} \cdot R)^3 \cdot c_{13} + c_{14}\right)$$

Constant	value	Constant	value
C_1	0.95328	C_8	0.85266
C_2	-0.389	C_9	-1
C_3	-17.057	C_{10}	0.77396
C_4	-2.9882	C_{11}	-18.266
C_5	-2.9887	C_{12}	0.95328
C_6	-0.27416	C_{13}	-0.007802
C_7	-0.088845	C_{14}	-0.095742

REFERENCES

1. Lide DR, CRC handbook of chemistry and physics. CRC press, 2004.