Supplementary Information

Molecular Dynamics Simulations of Liquid Gallium Alloy Ga-X (X=Pt, Pd, Rh) via Machine Learning Potential

Fang Fang,[1] Jie Lin,[1] Jiajia Li,[1] Yu Zhang,[1] Qiuyi Fu,[1] Quanquan Zhou,[1,2] Wei Li,[3] Guobing Zhou,*[,1,2] Zhen Yang*[,1,2]

[1]*Institute of Advanced Materials, College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang 330022, People's Republic of China*

[2]*State-Province Joint Engineering Laboratory of Zeolite Membrane Materials, National Engineering Research Center for Carbohydrate Synthesis, Key Lab of Fluorine and Silicon for Energy Materials and Chemistry of Ministry of Education, Jiangxi Normal University, Nanchang 330022, People's Republic of China*

[3]*Key Laboratory of Mesoscopic Chemistry of Ministry of Education, Institute of Theoretical and Computational Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, P. R. China*

*E-mail: gbzhou@jxnu.edu.cn (G.B. Zhou)

*E-mail: yangzhen@jxnu.edu.cn (Z. Yang)

1. Simulation details

Table S1. The cell sizes (unit: Å) for all studied systems in this work.

Temperatures	Systems (100 atoms)		
	Ga-Pt	**Ga-Pd**	**Ga-Rh**
400 K	12.44	12.44	12.44
600 K	12.52	12.52	12.52
800 K	12.61	12.61	12.61
1000 K	12.70	12.70	12.70
Temperatures	**Systems (300 atoms)**		
	Ga-Pt	**Ga-Pt**	**Ga-Rh**
400 K	17.94	17.94	17.94
1000 K	18.32	18.32	18.32

2. density of atomistic states of transition metal atoms

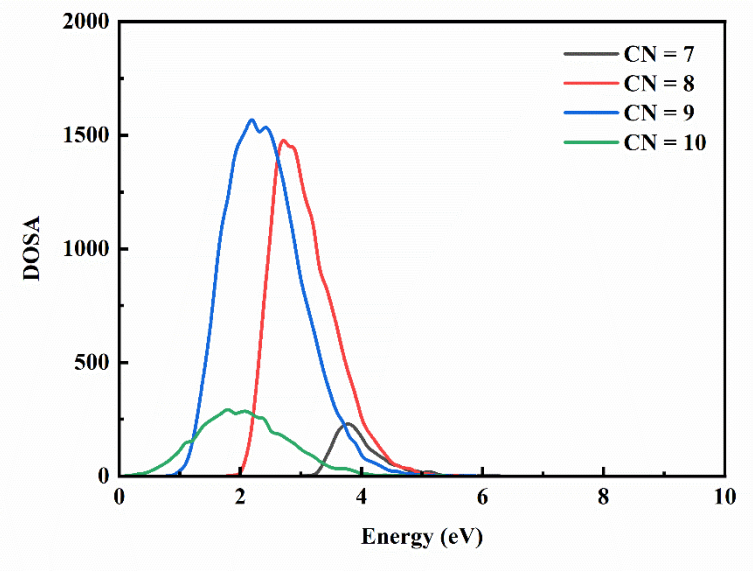

Figure S1. Density of atomistic states of Pt atom with different coordination number in Ga-Pt systems at 400 K.

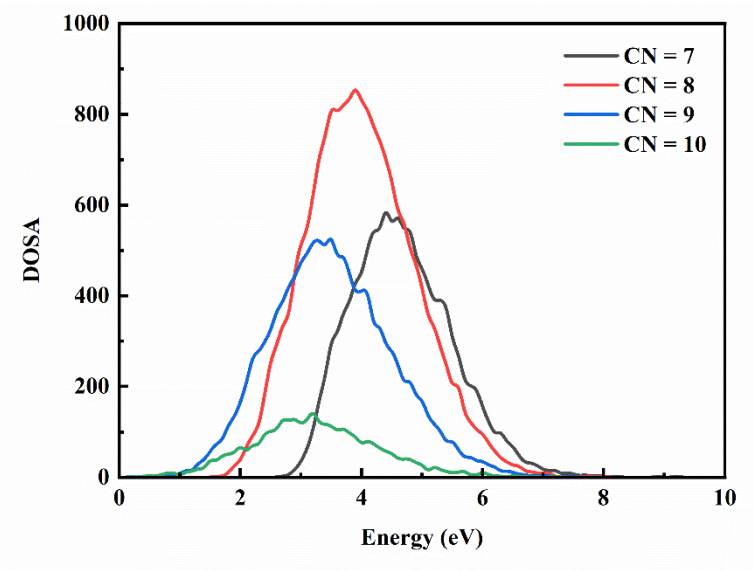

Figure S2. Density of atomistic states of Pt atom with different coordination number in Ga-Pt systems at 1000 K.

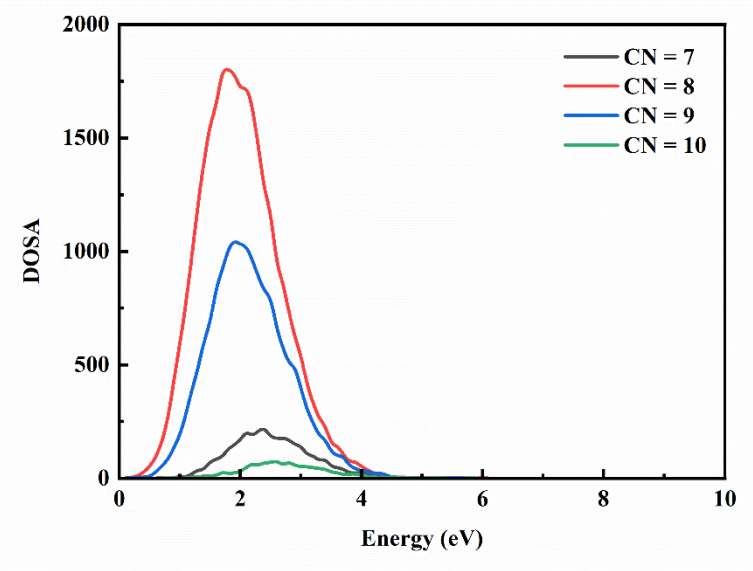

Figure S3. Density of atomistic states of Pd atom with different coordination number in Ga-Pd systems at 400 K.

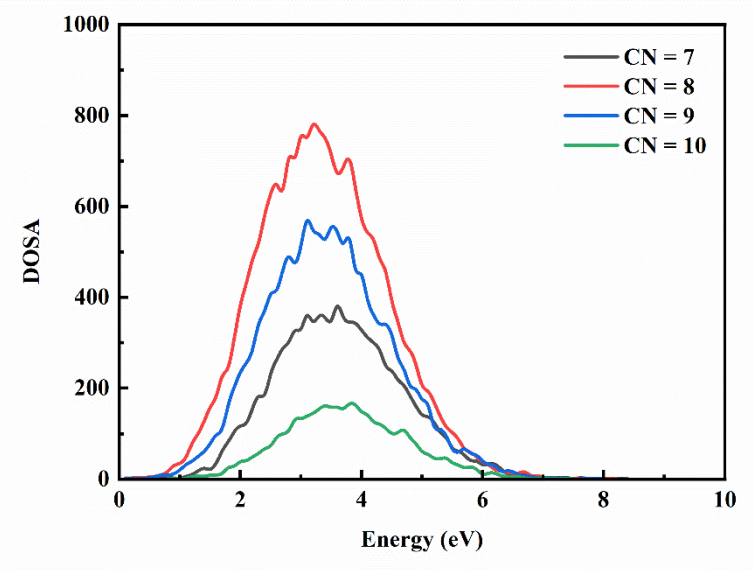

Figure S4. Density of atomistic states of Pd atom with different coordination number in Ga-Pd systems at 1000 K.

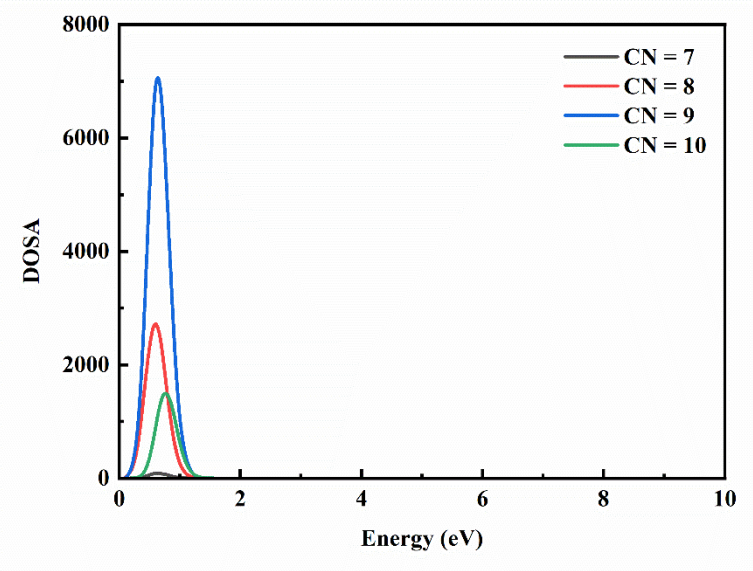

Figure S5. Density of atomistic states of Rh atom with different coordination number in Ga-Rh systems at 400 K.

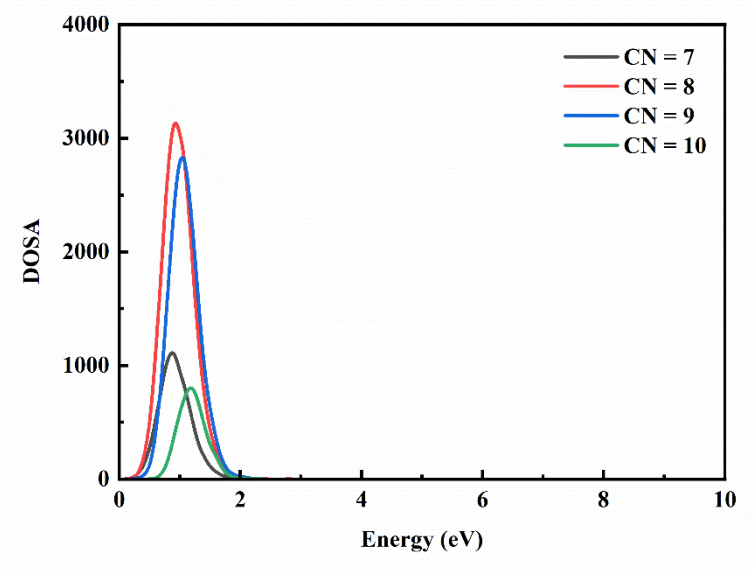

Figure S6. Density of atomistic states of Rh atom with different coordination number in Ga-Rh systems at 1000 K.

3. mean square displacement of transition metal atoms

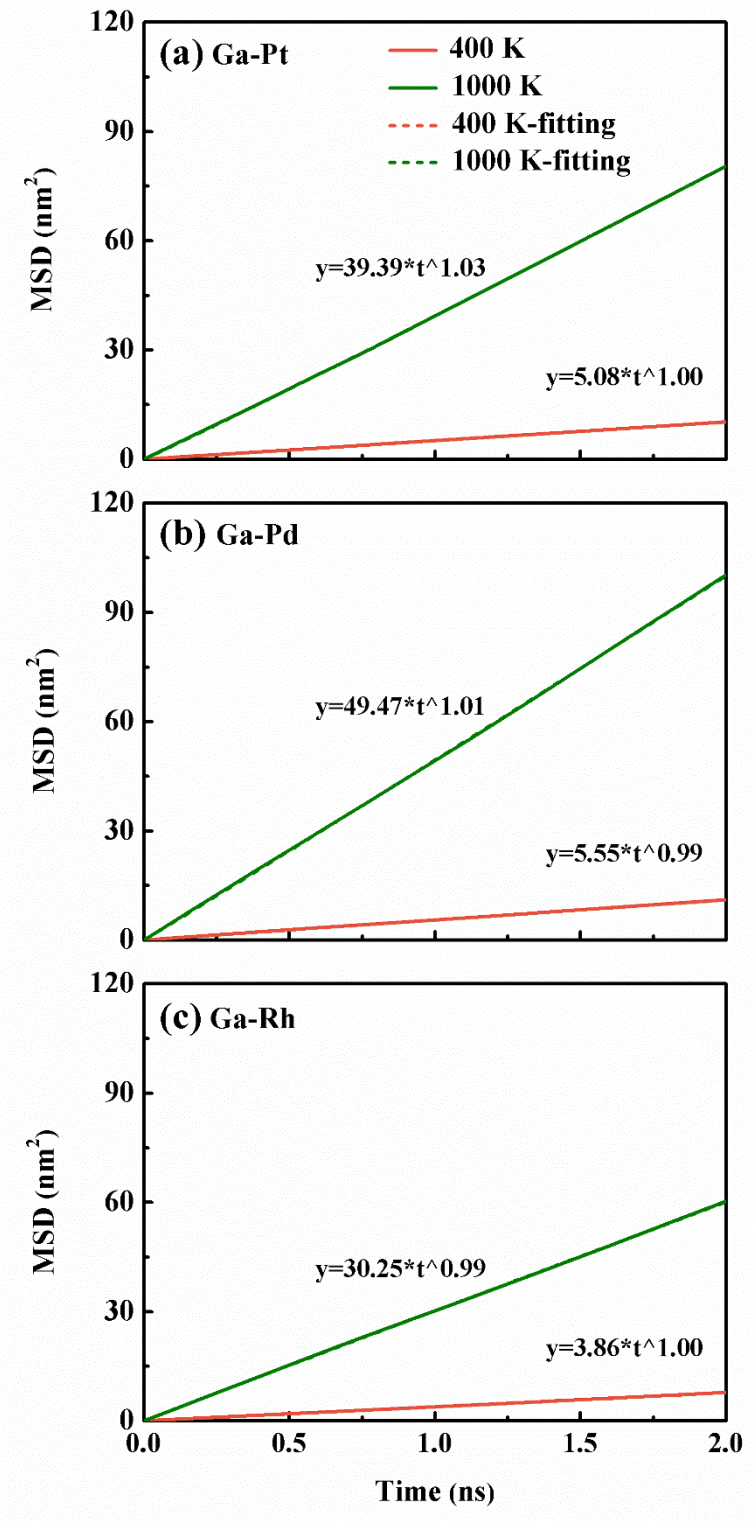

Figure S7. MSD and fitting curves ($y = a_0 \cdot t^{\alpha}$) for transition metal atom at different temperatures for three LGA systems: (a) Ga-Pt, (b) Ga-Pd, (c) Ga-Rh.

4. Diffusion barrier of transition metal atoms

We analyzed the free energy distributions of transition metal atom moving away from its neighboring Ga atoms by using the following expression: [S1,S2]

$$\Delta G(r) = -k_B T \ln g(r)$$

where g(r) represents the radial distribution function between X and Ga atoms. As shown in Figure 1, transition metal atom X needs to cross a high energy barrier (ΔG) when it diffuses away from its neighboring Ga atoms. At 400 K, the calculated ΔG values for Ga-Pt, Ga-Pd, and Ga-Rh systems are 12.75, 12.57, and 14.45 kJ/mol, respectively, while the counterparts at 1000 K are 17.64, 14.60, and 19.57 kJ/mol.

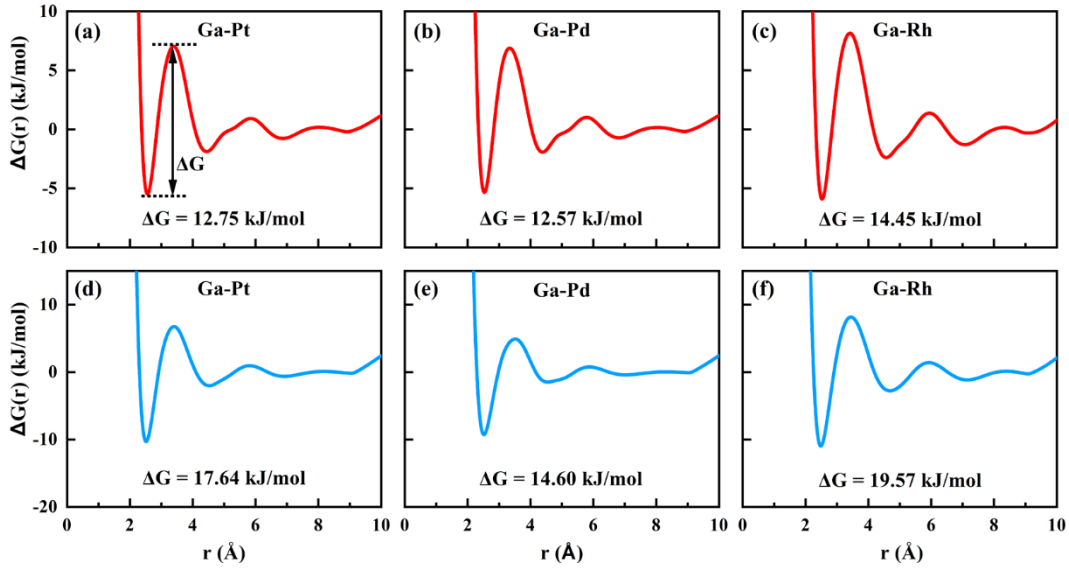

Figure S8. The free energy distribution profiles of transition metal atom X gradually moving away from its neighboring Ga atom in the systems of (a, d) Ga-Pt, (b, e) Ga-Pd, and (c, f) Ga-Rh at 400 K (upper panel) and 1000 K (lower panel).

References

S1 K. Tay, F. Bresme, Hydrogen Bond Structure and Vibrational Spectrum of Water at a Passivated Metal Nanoparticle. *J. Mater. Chem.*, 2006, **16**, 1956–1962.

S2 Andrew R. Leach, Molecular modeling: principles and applications, 2nd ed., Pearson Education, Harlow, 2001.