Supplementary Information

Mechanistic Study of the Adsorption Capabilities of Heavy Metals on the Surface of Ferrihydrite：Batch sorption, modeling and Density Functional Theory

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The supporting information provides additional tables and figures showing: Applying the parameters of mono-systems to a multi-system (Fig. S1). The Eads and atomic configuration of Zn^{2+} adsorption on different sites of Fh(103) surface (Fig. S2). The Eads and atomic configuration of Ni^{2+} adsorption on different sites of Fh(103) surface (Fig. S3). The Bader charge of Pb^{2+}, $Zn^{2+,}$, $Ni^{2+}$and O in all adsorbed models (Table S1). The bond lengths between the adsorbed ions and the Fh surface (Table S2).

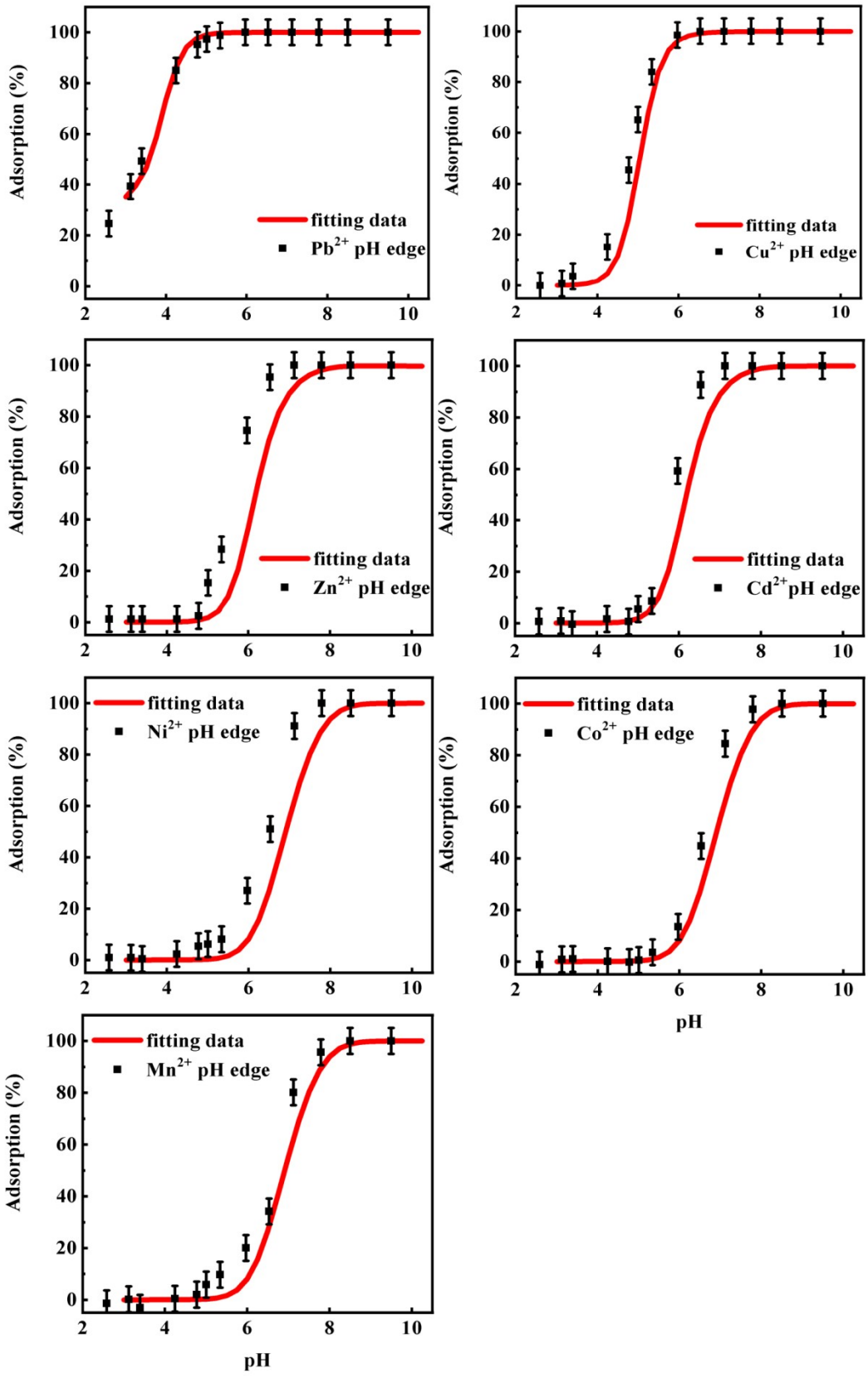
Adsorption (%)
fitting data
Pb2+ pH edge
Cu2+ pH edge
Zn2+ pH edge
Cd2+pH edge
Ni2+ pH edge
Co2+ pH edge
Mn2+ pH edge
pH

Fig. S1 Applying the parameters of mono-systems to a multi-system

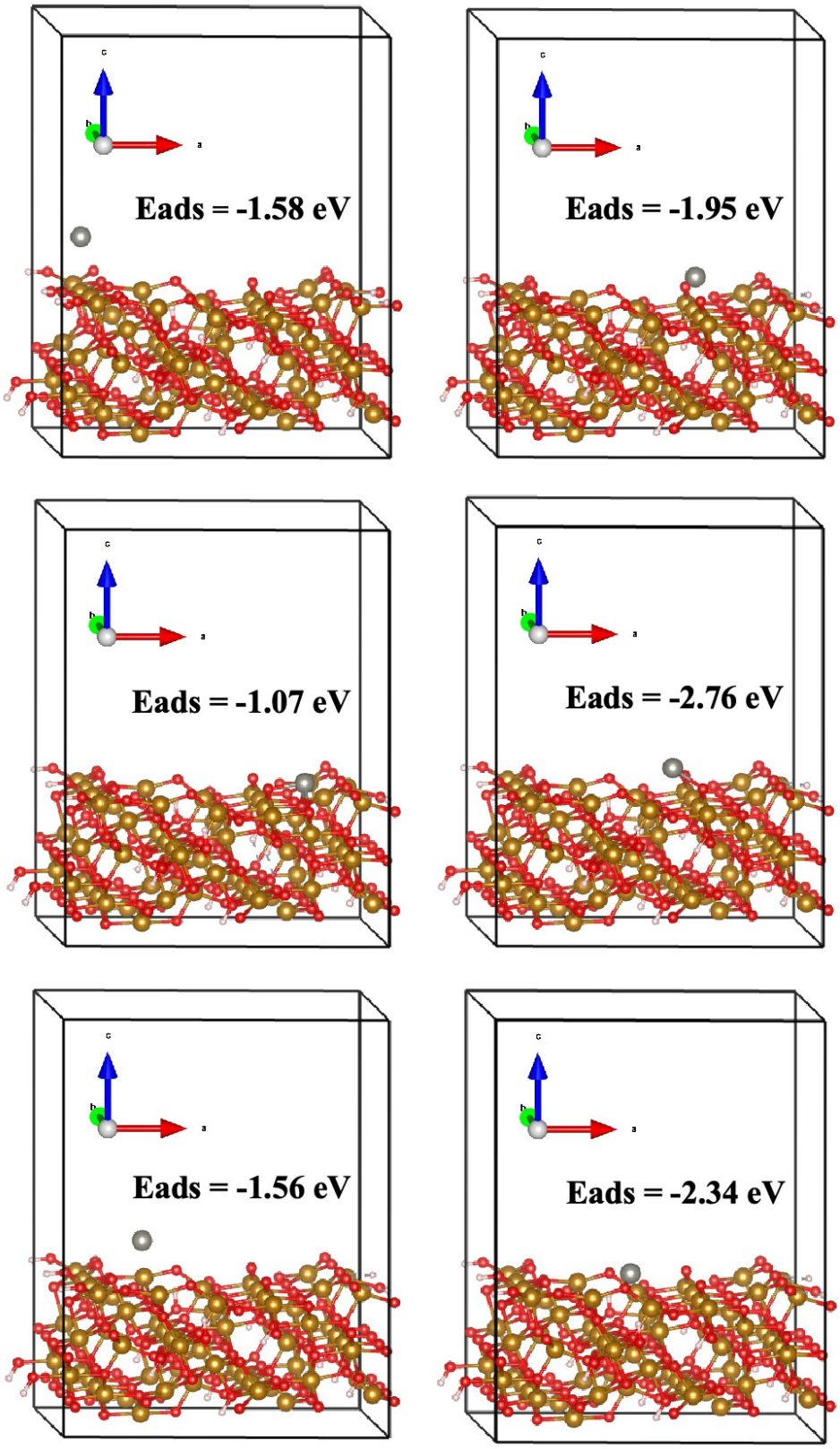

Fig. S2 The Eads and atomic configuration of Zn^{2+} adsorption on different sites of Fh(103) surface

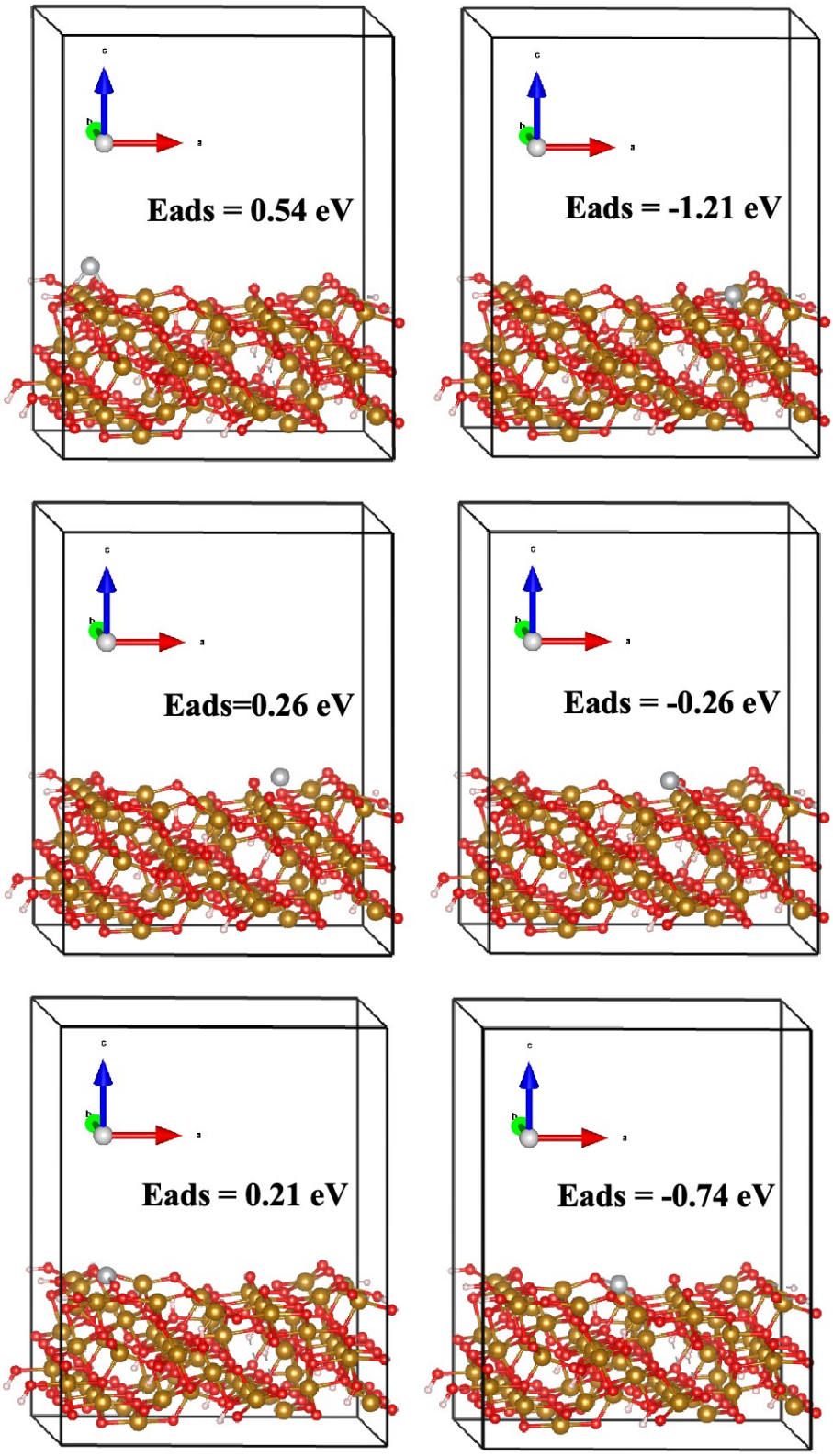

Fig. S3 The Eads and atomic configuration of Ni^{2+} adsorption on different sites of Fh(103) surface

Table S1 The Bader charge of Pb^{2+}, $Zn^{2+,}$, $Ni^{2+}$and O in all adsorbed models

	O	Pb	Zn	Ni
Fh(103)-Pb	-0.94	0.94		
Fh(103)-Zn	-0.72		0.72	
Fh(103)-Ni	-0.63			0.63

Table S2 The bond lengths between the adsorbed ions and the Fh surface.

Adsorbed Ion	Bond Length(Å)
Pb-O	2.45 ± 0.08
Zn-O	2.73 ± 0.06
Ni-O	2.92 ± 0.05