Supplementary Materials for

Insights into the ion-exchange properties of Zn(II)-incorporated MOR zeolites for the capture of multivalent cations

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Experimental S1. Synthesis of Al-MOR with different Si/Al ratio.

Synthesis of Al-MOR gel is described in the experimental section in the manuscript. For Al-MOR-1 and Al-MOR-2, the chemical compositions of the gel mixtures (without seed crystals) were 3.68Na_2O: 1 Al_2O_3: 16.0 SiO_2: 240H_2O. The seed crystals content was fixed at 10 wt.% on a basis of SiO_2. The mixture was placed in a 60mL reactor at 423 K and hydrothermal reacted for 96 hours (Al-MOR-1) and 48 hours (Al-MOR-2), respectively. For Al-MOR-3, the chemical composition of the gel mixtures (without seed crystals) was 2.76Na_2O: 1 Al_2O_3: 12.0 SiO_2: 180H_2O. The seed crystals content was fixed at 10 wt.% on a basis of SiO_2. The mixture was placed in a 60mL reactor at 423 K and hydrothermal reacted for 96 hours. After all the reaction was completed, the sample was filtered and washed to neutrality and dried in an oven at 353 K for further use.

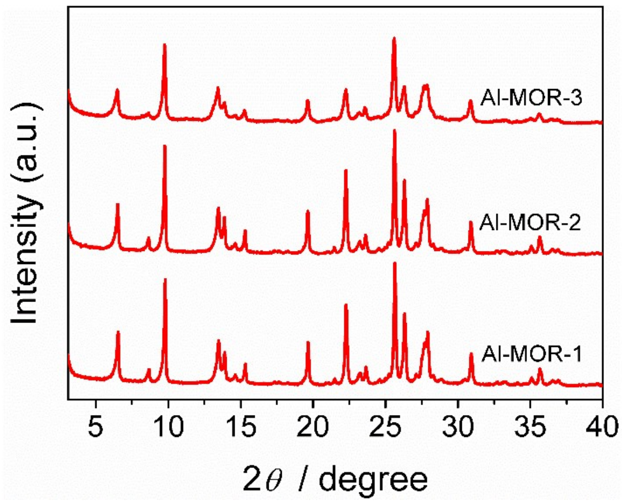

Fig.S1. XRD patterns of various Al-MOR.

As shown in Fig. S1, the XRD patterns suggest that all the materials synthesized were pure MOR zeolites. Furthermore, the compositions of the three MOR zeolites were analyzed by ICP-AES. As shown in Table S1, the Si/Al ratio decreased from Al-MOR-1 to Al-MOR-3, and the charge density (Al/Si ratio) increased from Al-MOR-1 to Al-MOR-3.

Table S1. Compositions of various Al-MOR.

	Si/Al	Na/Al	Al/Si
Al-MOR-1	5.87	1.08	0.17
Al-MOR-2	5.69	1.03	0.18
Al-MOR-3	4.81	1.06	0.21

Experimental S2. Synthesis of Zn,Al-MOR with different zinc content.

Synthesis of Zn,Al-MOR gels is described in the experimental section in the manuscript. For Zn,Al-MOR with Zn/(Zn+Al)=0.6 (Here after denoted as Zn0.6, which denoted as Zn,Al-MOR in the manuscript), the chemical composition of the gel mixtures (without seed crystals) was $1.84Na_2O$: $0.2Al_2O_3$: 0.6ZnO: $8.0SiO_2$: $120H_2O$. The seed crystals content was fixed at 10 wt.% on a basis of SiO_2. For Zn,Al-MOR with Zn/(Zn+Al)=0.4 (Here after denoted as Zn0.4), the chemical composition of the gel mixtures (without seed crystals) was $1.84Na_2O$: $0.3Al_2O_3$: 0.4ZnO: $8.0SiO_2$: $120H_2O$. The seed crystals content was fixed at 10 wt.% on a basis of SiO_2. All the mixtures were placed in 60 mL reactor at 423 K and hydrothermal reacted for 72 hours. After the reaction was completed, the sample was filtered and washed to neutrality and dried in an oven at 353 K for further use.

The effect of zinc content on ion exchange properties was studied. Fig. S2 was the XRD patterns of Zn0.4 and Zn0.6, both were pure MOR zeolites. The comparison of ion exchange properties between Zn0.4 and Zn0.6 was studied. As shown in Fig. S3a, the kinetics for Ni^{2+} suggest that both Zn0.4 and Zn0.6 can reach ion exchange equilibrium with 3 days. Herein, further ion exchange experiments were conducted for 3 days. The isotherms shown in Fig. S3b revealed that Zn0.6 has much better selectivity and efficiency for exchanging Ni^{2+} than Zn0.6. Considering that Zn0.6 has higher zinc content than Zn0.4, it can be concluded that the increase of zinc in MOR framework can benefit the ion exchange properties.

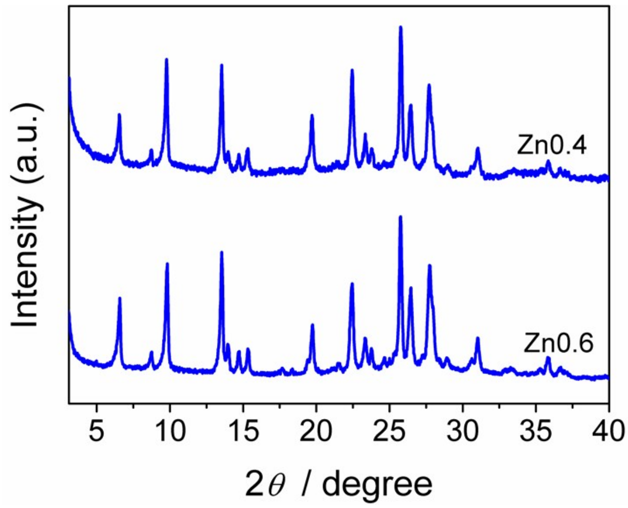

Fig. S2. XRD patterns of Zn0.4 and Zn0.6

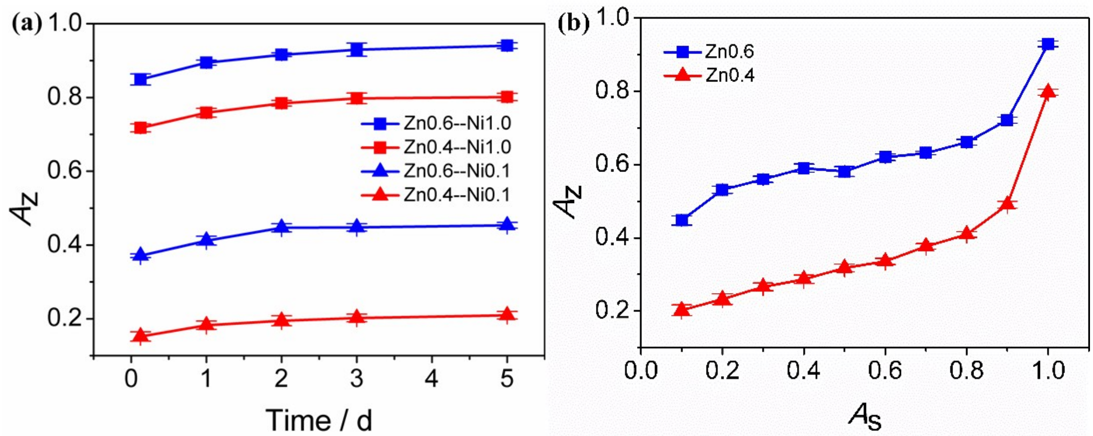

Fig. S3. Ion exchange kinetics (a) and isotherms (b) for Ni^{2+}.

Experimental S3. Ion exchange properties for Rb^+

The ion exchange property of Zn,Al-MOR and Al-MOR for monovalent cation was studied by using Rb^+ as target cation. The ion exchange kinetics and isotherms for Rb^+ were shown in Fig. S4. The kinetics in Fig. S4a suggested the ion exchange for Rb^+ all reached equilibrium within 2 days. Therefore, the ion-exchange isotherms were obtained by conducting for 2 days to obtain each point (Fig. S4b). The results indicated that ion exchange efficiency of Al-MOR for Rb^+ is better than that of Zn,Al-MOR, which probably because stabilization of two Rb^+ cations by the two negative charge generated by Zn in the close environment is hindered by the structure constrain. Furthermore, the ion exchange isotherms at different temperatures were studied. As shown in Fig. S5, the isotherms suggest both Zn,Al-MOR and Al-MOR show a slight temperature dependence for exchanging Rb^+. Moreover, the XRD pattern shown in Fig. S6 suggested that the structures of MOR zeolites were maintained after Rb^+ exchange.

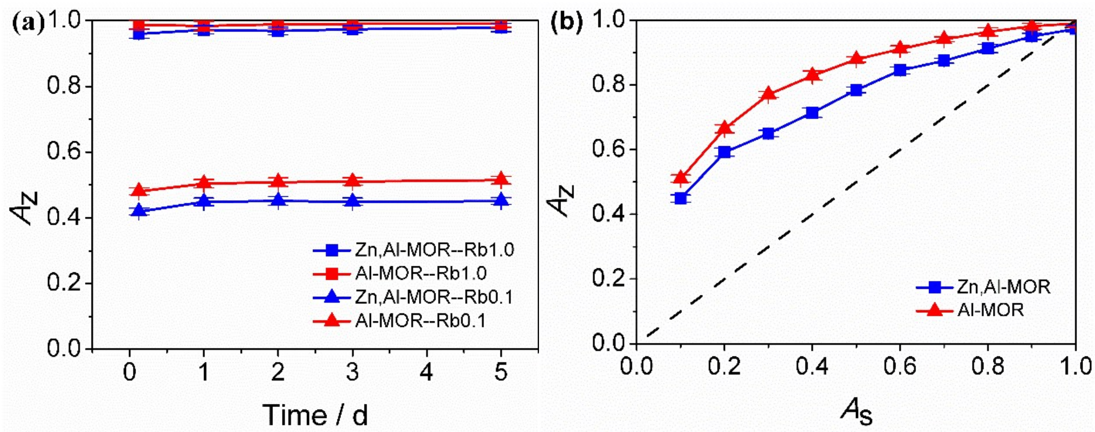

Fig. S4. Ion exchange kinetics (a) and isotherms (b) for Rb^+.

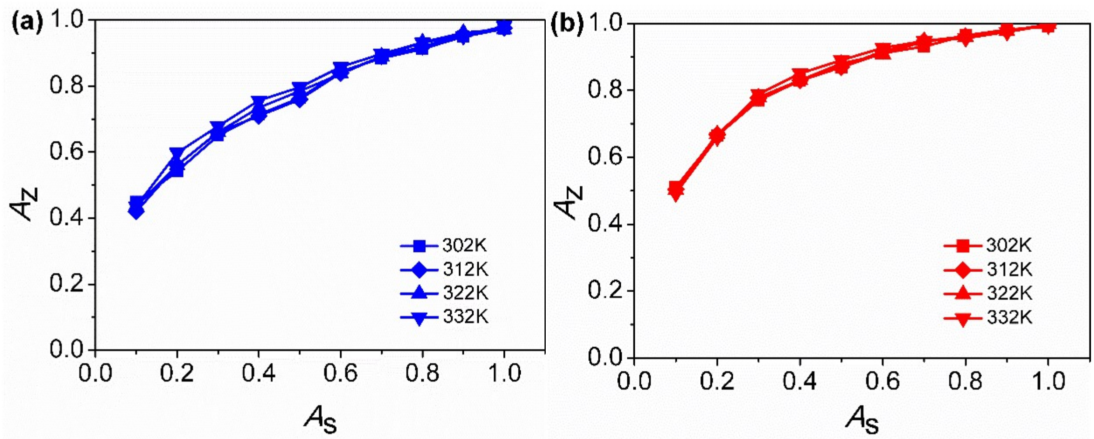

Fig. S5. Temperature dependence of ion exchange isotherms for Rb^+: (a) Zn,Al-MOR, (b) Al-MOR.

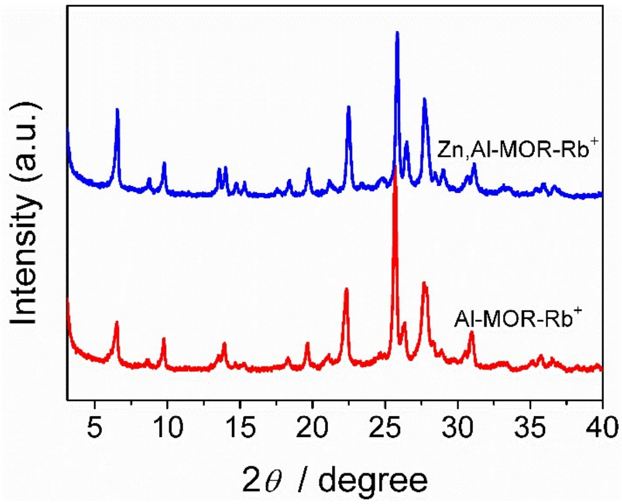

Fig. S6. XRD patterns after Rb^+ ion exchange.