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Separating 3d-elements by reactive nanopores within functionalized zirconium-based metal-organic framework

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Recycling and separating critical minerals (CM) such as manganese (Mn2+), cobalt (Co2+) and nickel (Ni2+) from electronic wastes can help secure the global critical mineral (CM) supply and clean energy production. Metal-organic frameworks (MOFs) are a promising material class to effectively sequester CMs from heterogeneous aqueous solutions due to their large surface areas, large pore volumes and size, and tunable reactivities. Functionalization of MOFs can modify the ion-binding properties of these materials, prompting the metal-specific chemical chelation towards target CMs, enhancing the sequestration capacity. Zirconium-based MOF (MOF-808) was investigated for its selective adsorption behavior in the absence and presence of nitrogen containing functional groups, pyrazole (MOF-808-PyC). Pristine MOF-808 shows an adsorption trend of Mn2+ > Co2+ ≈ Ni2+ while this trend changes for MOF-808-PyC, showing the increased selectivity towards Ni2+ followed by Mn2+ and Co2+. This result suggests i) the sorption mechanisms are different between MOF-808 and MOF-808-PyC which can be metal specific and ii) pyrazole has stronger affinity to Ni2+ over Co2+ and Mn2+. X-ray absorption fine structure spectroscopy (XAFS) indicates that Ni2+ has a similar local coordination environment in the pristine MOF-808 and in pyrazole-functionalized MOF-808-PyC. XAFS shows that Ni2+ coordinates to the Zr-metal oxo-cluster. Furthermore, X-ray photoelectron spectroscopy indicates that electronic environment around nitrogen changes with Ni2+ adsorption, unambiguously indicating that nitrogen-containing groups, such a pyrazole, impact the selectivity of MOF-808. This likely indicates, that there are several types of surface complexation for Ni2+ in MOF-808. Our study provides important scientific insights for the design of new materials for ion separations that are relevant for CMs recycling, specifically for cathode recycling from lithium ion batteries.
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References

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