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# Surface acidity and metal complexation of edges of birnessite: a first principles approach

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Birnessite, a layered $MnO_2$ mineral, is ubiquitous in many natural environments and plays a key role in adsorbing and fixing trace elements. The basal surface (i.e. (001)) has received remarkable attentions. Recently, increasing evidence indicates that the edge surface is more reactive than the basal surface. Due to the presence of various amphoteric groups, edge surfaces show pH-dependent interfacial properties. In this study, we carried out first principles calculations on surface acidity (pKas) and metal complexation of birnessite edge surface. By using first principles molecular dynamics (FPMD) based vertical energy gap technique, we derived pKas of birnessite (010) edge and thus identified the active sites for complexing metal cations. We then investigated the adsorption and incorporation of metal cations including transition metal cations (such as $Ni^{2+}$, $Zn^{2+}$) and rare earth elements (REEs such as $Sc^{3+}$, $Y^{3+}$, $La^{3+}$). Comparison will be made with clay minerals (i.e. phyllosilicates) and the difference will be presented. The results in this study provide an atomic scale view of interfacial processes of birnessite.