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| Title | First principles calculations study of α-MnO2 as a potential cathode for Al-ion battery application. | | |
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| Abstract |  |
| α-MnO2 is considered as an attractive cathode material for lithium, sodium and magnesium-ion battery applications because of its relatively large [2 × 2] tunnel, high discharge capacity, environmental benignity and low cost. Therefore, understanding the electrochemical properties of α-MnO2 for eco-friendly trivalent aluminum-ion battery is of great research interest. Herein, we presented a theoretical study of Al insertion into α-MnO2 using first principles calculations based on the density functional theory. We found that Al insertion into α-MnO2 proceeded through 4 insertion stages. The average calculated voltage was found to be 1.55 V. Moreover, our calculations suggested the structural distortion of α-MnO2 upon Al insertion even in the dilute limit of insertion. In addition, the electronic properties of the Al-inserted phases and the effect of the metal doping strategy in α-MnO2 for performance improvement were also discussed. Our study may provide an insight and pave the way for further applications of α-MnO2 as an electrode material and potential insertion host for aluminum-ion batteries. | |