Contribution ID: **125** Type: **Poster Presentation**

Ab-Initio study of Oxygen Adsorption on Li/Na-MO₂ (110) Surface, (M = Mn,Ti and V)

Tuesday, 4 July 2017 17:10 (1h 50m)

Metal air batteries have been studies extensively but operation of Na-air batteries has just gained attention recently. Catalytic effect on the performance of sodium air battery has not been an area of interest yet. However, it has been reported that the most stable product in Na-air battery is NaO₂ whereas in Li-air battery it has been reported that the major and stable product is Li₂O₂. In this paper, we present density functional theory study on how metal oxide (MnO₂, TiO₂ and VO₂) catalyst affects the formation of Li₂O₂ and NaO₂ and other products that may be formed. We further investigate the discharge products of these two metal air batteries compared to the known systems of the product in terms of their formation energy and their morphology. Looking into the O-O bond length which plays an important role in Oxygen Reduction Reaction (ORR) during discharge of the battery. Interestingly it has been found that what was reported in literature, that the most stable products in Na-air batteries being NaO₂ is indeed what has been observed in our study. Furthermore, the type of structure that has been found was the pyrite form whereas the most stable product in Li-air battery, Li₂O₂ has the hexagonal type. Amongst the three metal oxides it can be concluded that MnO₂, is the most favourable catalyst because it encourages the formation of the reported stable products in both metal air batteries.

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