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Computational investigation of vacancy ordering in gamma-Mn₂O₃.

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A high energy demand as a result of a growth in living standards and population has stimulated the efforts to develop high energy density power sources which is, metal air batteries. However, the fundamental challenge that limits the use of metal air battery technology is the ability to find a catalyst that will catalyse Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER). Density Functional study was employed to investigate the ordered tetragonal structure using a supercell of the cubic structure Mn₃O₄. We obtain the spectrum of energies of all the ordered configurations which contribute to the partially disordered Mn₂O₃ structure. The degree of ordering in manganese vacancies in the octahedral sites appears to be more stable than the in tetrahedral manganese.

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