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COMPUTATIONAL MODELLING STUDY ON PHASE STABILITY OF TiO₂ and MnO₂

Energy is the basis of societies' welfare, economic and development. Population growth, industrial development, and economic growth lead to increased energy demand. Due to their high energy and long cycling life, lithium-ion batteries have held a significant share of the energy storage market for portable electronics and electric vehicles. However, with the rapid development of renewable energy plants, there is an urgent demand for energy storage systems with exceptionally good cycling performance, high safety and low cost. Discovering materials to improve the safety and power density of existing Li-ion batteries is important, here we consider a study on TiO2 and MnO2. In the current work we present a comparative study on structural, mechanical, vibrational and electronic properties of TiO2 and MnO2 investigated using ab initio method within density functional theory. Lattice parameters for the materials are in good agreement with experimental values to 5%. The heats of formations suggest that the structures are stable with negative values. Elastic properties indicates that the structures are mechanically stable due to positive elastic constant and satisfying necessary mechanical stability criteria condition for tetragonal structure. UNCLE code and Monte Carlo simulation was used to determine 36 phases of mixed Ti-MnO2 system.
Keywords: Energy storage, Lithium-battery, ab initio, Phase stability

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