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Electronic Stability and Surface Study of Tin Dioxide

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In lithium-air batteries, metal oxides are frequently regarded as excellent catalysts that help produce stable discharge products and deliver better electrochemical performance. The metal-air battery is a type of electrochemical cell or battery that generates electricity by oxidizing a metal, such as Li, K, Na, or Mg, at the anode and reducing oxygen at the cathode. In this study, we use the density functional theory calculation to investigate the bulk properties and surfaces stability of tin dioxide. Tin dioxide was found to be a stable semiconductor with a band gap of 0.63 eV. The phonon dispersion curves indicate that the structure is vibrationally stable since it shows no soft mode along the brillouin zone direction. The elastic constants show that our structure is mechanically stable since the C' is positive and obey the mechanical stability criteria for a tetragonal crystal. Furthermore, we modelled the low Miller index surfaces which are (110), (101), (111), (001) and (100) from the fully optimised bulk structure using METADISE code. From the modelled surfaces, (110) had the lowest surface energy which is in agreement with the reported literature. The addition of two oxygen atoms revealed the most stable adsorption energy is the bridging configuration was the most favourable. This study will lead to understanding if tin dioxide will catalyse the oxygen reduction reaction in metal air batteries

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

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