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Crystal and electronic structures of $Li_2Ti_6O_{13}$ for lithium-ion batteries

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The valuable non-renewable resources such as petroleum and natural gas will gradually peter out in near future, therefore alternative sources of energy are becoming of increasing interest. Moreover, in order to store energy, rechargeable lithium batteries are of particular interest since they have a possibility for portability and together with a high conversion efficiency. Hexa-titanium oxide based materials, such as $Na_2Ti_6O_{13}$, $K_2Ti_6O_{13}$ or $Li_2Ti_6O_{13}$, have been intensively investigated because of their potential applications as electrodes for ion-exchange batteries. By means of first-principles calculations, we study the electronic structure of $Li_2Ti_6O_{13}$, which has been experimentally shown as one of possible materials for a cathode in lithium-ion batteries. We have obtained the crystal structure of $Li_2Ti_6O_{13}$ and Ti_6O_{13}, which Ti_6O_{13} was not completely determined experimentally. The overall lattice parameter are quite good agreement with experimental. Our calculated band gap of $Li_2Ti_6O_{13}$ is 2.92 eV when a general gradient approximation (GGA) functional were used, while the experimental band gap is 3.5 eV. The electronic band dispersion reveals that the both electron and hole mobility are low. The capability to store energy can be expressed in term of intercalation voltage. Our computational average intercalation voltages are 2.08 Volt with GGA-PBE functional and 1.78 Volt with HSE Hybrid functional. Our calculation are found to be in excellent agreement with experiments of 1.70 Volt.

Summary

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