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First Principles Study for Lithium Intercalation and Diffusion Behavior in Orthorhombic Nb2O5 Electrochemical Supercapacitor CHI-PING LIU, FEI ZHOU, VIDVUDS OZOLINS, University of California, Los Angeles — Unlike batteries, electrochemical supercapacitors require not only high energy density, but also very fast rates of electronic and ionic transport. Experimental results show that niobium oxide exhibits an outstanding power density and fast ionic charging rates. We investigate lithium intercalation and diffusion behavior in orthorhombic niobium oxide (T-Nb2O5) by using first-principles density-functional theory (DFT) calculations. We find that the Li ions can only intercalate in the 001 family of lattice planes with the lowest niobium occupancy due to electrostatic-repulsion between Li+ and Nb5+. Besides, since Li diffusion along the z direction is hindered by a high diffusion barrier (2.64 eV), the overall Li intercalation and diffusion can only occur within 001 planes. Furthermore, the diffusion barriers within the 001 planes are found to have a broad distribution of values form around 50 meV to 1000 meV; the diffusion barrier is determined by the neighboring oxygen-oxygen distance. The barrier remains low (around 60 meV) when the neighboring oxygen distance along the diffusion path is larger than 3.9 Å, thus leading to fast Li ion diffusion. These results explain the excellent performance of Nb2O5 as a cathode material for electrochemical supercapacitors.

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