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First principles studies of structure stability and lithium intercalation of ZnCo2O4 YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center, WEIWEI LIU, Beijing Computational Science Research Center, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER TEAM — Among the metal oxides, which are the most widely investigated alternative anodes for use in lithium ion batteries (LIBs), binary and ternary transition metal oxides have received special attention due to their high capacity values. ZnCo2O4 is a promising candidate as anode for LIB, and one can expect a total capacity corresponding to 7.0 - 8.33 mol of recyclable Li per mole of ZnCo2O4. Here we studied the structural stability, electronic properties, lithium intercalation and diffusion barrier of ZnCo2O4 through density functional calculations. The calculated structural and energetic parameters are comparable with experiments. Our theoretical studies provide insights in understanding the mechanism of lithium ion displacement reactions in this ternary metal oxide.

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