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BC_3 as electrode for Mg ion batteries[1] RAJENDRA JOSHI, Science of Advanced Materials, Central Michigan University, VERONICA BARONE, JUAN PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University — We propose layered BC_3 a novel electrode material for rechargeable magnesium ion batteries. Using dispersion-corrected density functional theory calculations, we show that layered BC_3 can intercalate Mg ions between its layers to form the stoichoimetry $Mg_{0.5}BC_3$, which corresponds to a theoretical capacity of 572 mAh/g. We also propose a three step staging mechanism for Mg ion intercalation in BC_3 and show that it presents a moderate open circuit voltage in the range of 0.82 to 0.96 V with respect to metallic Mg anode.

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