

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Hexagonal  $\text{BC}_3$  as a Robust Electrode Material for Li, Na, and K Ion Batteries**<sup>1</sup> RAJENDRA JOSHI, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, BURAK OZDEMIR, Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JUAN PERALTA, VERONICA BARONE, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA — We propose hexagonal  $\text{BC}_3$  as a robust electrode material for Li, Na, and K ion batteries based on first-principles density functional theory calculations. We show that, by intercalating Li, Na, and K in  $\text{BC}_3$ , it is possible to form  $\text{Li}_{1.5}\text{BC}_3$ ,  $\text{Na}_1\text{BC}_3$ , and  $\text{K}_{1.5}\text{BC}_3$  which correspond to a high theoretical capacity of 858 mA h/g, 572 mA h/g, 858 mA h/g, respectively. In addition, this material presents small open circuit voltage variations of 0.49, 0.12, and 0.16 V when used as electrode for Li, Na, and K ion batteries, respectively.

<sup>1</sup>NSF CBET-1335944, NSF DMR-0906617, DOE DE-FG02-10ER16203

Rajendra  
Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 4

Date submitted: 06 Nov 2015

Electronic form version 1.4