

Electronic Supporting Information (ESI)

Electrolytic Calcium Hexaboride for High Capacity Anode of Aqueous Primary Batteries

Huayi Yin,^[a,b] Diyong Tang,^[a] Xuhui Mao,^[a] Wei Xiao,^{*[a]} and Dihua Wang^{*[a]}

[a]School of Resource and Environmental Science, Wuhan University, 430072,

Wuhan, P. R. China. Fax/Tel: 008627 6877 4216; E-mail: wangdh@whu.edu.cn

[b] Department of Materials Science and Engineering, Massachusetts Institute of Technology,

Cambridge, 02139 MA, USA

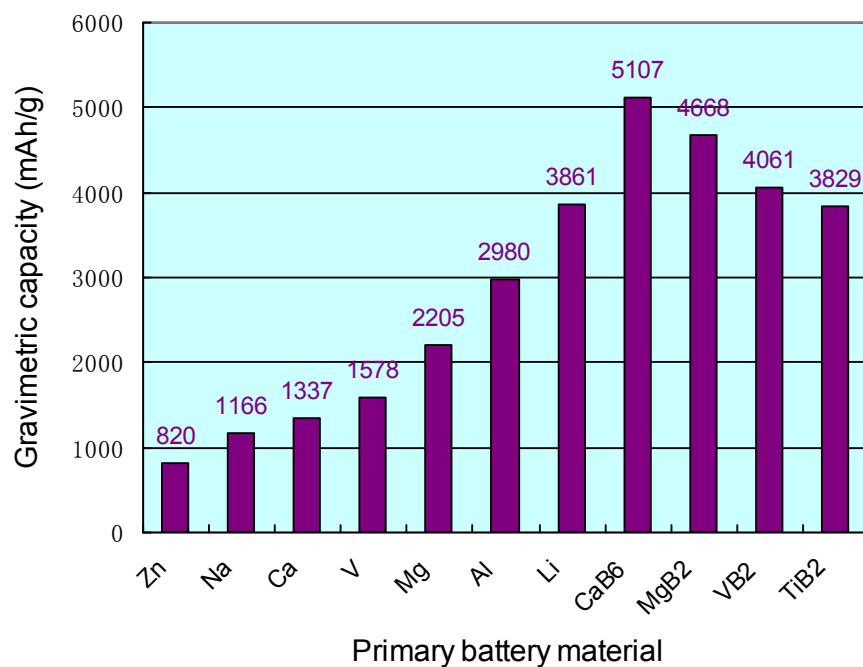


Figure S1. Theoretical gravimetric capacity of potential primary anode materials.

Table S1. Decomposition voltage of calcium borate in molten CaCl₂-NaCl at 600°C

Reactions (600 °C)	E(V)
2CaB ₂ O ₄ = Ca ₂ B ₂ O ₅ + 2B + 1.5O ₂ (g)	1.877
3CaB ₂ O ₄ = Ca ₃ B ₂ O ₆ + 4B + 3O ₂ (g)	1.896
6Ca ₂ B ₂ O ₅ = 4Ca ₃ B ₂ O ₆ + 4B + 3O ₂ (g)	1.952
5CaB ₂ O ₄ = 2Ca ₂ B ₂ O ₅ + CaB ₆ + 5O ₂ (g)	1.962
4CaB ₂ O ₄ = Ca ₃ B ₂ O ₆ + CaB ₆ + 5O ₂ (g)	1.973
CaB ₂ O ₄ = 2B + CaO + 1.5O ₂ (g)	2.016
8Ca ₂ B ₂ O ₅ = 5Ca ₃ B ₂ O ₆ + CaB ₆ + 5O ₂ (g)	2.017
3CaB ₂ O ₄ = CaB ₆ + 2CaO + 5O ₂ (g)	2.045
Ca ₂ B ₂ O ₅ = 2B + 2CaO + 1.5O ₂ (g)	2.156
3Ca ₂ B ₂ O ₅ = CaB ₆ + 5CaO + 5O ₂ (g)	2.17
Ca ₃ B ₂ O ₆ = 2B + 3CaO + 1.5O ₂ (g)	2.258
3Ca ₃ B ₂ O ₆ = CaB ₆ + 8CaO + 5O ₂ (g)	2.262
2NaCl = 2Na(l) + Cl ₂ (g)	3.226
CaCl ₂ = Ca + Cl ₂ (g)	3.437