Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First principle calculations of discharge curves of organic batteries with organic carbonyl compounds JOSIANE GAUDREAU, VÉRONIQUE BROUSSEAU COUTURE, MICHEL CÔTÉ, Univ of Montreal — The issue of intermittence in the production of energy from renewable sources could be alleviated using efficient/cost effective electrical storage facilities. Particularly, the organic batteries represent a green solution to this problem because of their potential low cost. The use of carbonyl materials as organic cathodes wields good results in terms of voltage and theoretical capacity for such batteries. The aim of this project is to predict the discharge curves of organic cathode batteries using first principle calculations. We use DFT results to predict the voltage of experimentally-tested materials for different redox stages. We study multiple methods, including different functionals (B3LYP and PBE) and implicit solvation model (SMD and PCM) to find which ones are most suitable for prediction purposes on a range of carbonyl compounds.

Josiane Gaudreau
Univ of Montreal

Date submitted: 10 Nov 2016 Electronic form version 1.4