Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study of amorphous carbon: a promising candidate for Na-ion batteries KONSTANTINOS KOTSIS, FLEUR LEGRAIN, SERGEI MANZHOS, National University of Singapore — The perspective of a widespread use of clean but intermittent sources of electricity (wind and solar) as well as that of hybrid electric vehicles calls for alternatives to Li-ion batteries as Li resources are limited. Na being abundant, cheap, and a relatively light and small atom, Na-ion batteries have attracted a lot of interest the past few years. However, while most of the Na-ion batteries studies focus on the positive electrode, the negative electrode remains little investigated and an efficient anode providing all a good capacity, a high cycle life, and a descent rate of charge/discharge, is still not available. The efficient electrode materials for Li, in particular diamond Si and graphite C, have been shown to not allow the intercalation of Na [1, 2]. Computational studies report positive intercalation energies [3, 4] and therefore suggest that the insertion of Na into the crystalline framework (C and Si) is thermodynamically not favored: Na atoms prefer to gather into Na clusters rather than to intercalate into the crystalline phase. Amorphization of Si was found to be a valid strategy to improve the interaction between Si and Na [3]. We investigate here the effects of amorphization of C on its storage properties vis-à-vis Na (as well as Li for reference).

Konstantinos Kotsis
National University of Singapore

Date submitted: 10 Nov 2014 Electronic form version 1.4