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Amorphous Carbon Is a Promising Material for Sodium Ion Battery Anodes: a Computational Study

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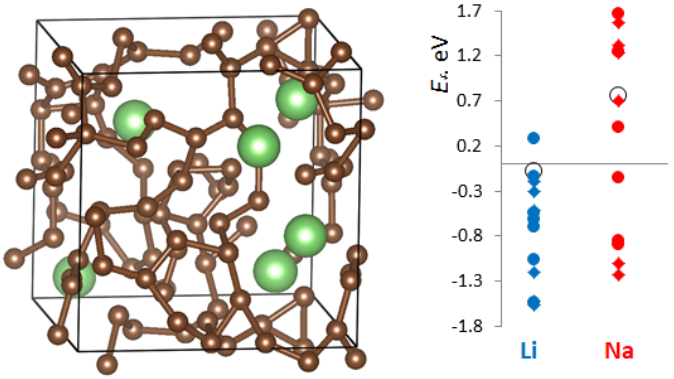
Sodium-ion batteries have recently attracted much interest. However, while most studies of Na-ion batteries focus on the positive electrode, the negative electrode remains less investigated and an efficient anode providing all a good capacity, a high cycle life, and a descent rate of charge/discharge, is still not available. The efficient electrode materials for Li, in particular crystalline Si and graphite C, have been shown to not allow the intercalation of Na.

Amorphization of Si has recently been shown to improve substantially the interaction between Si and Na, and amorphous Si (*a*-Si) has been predicted to allow Na insertion by two independent studies [1, 2]. Here, we show that the same holds for amorphization of carbon. Carbon is widely used as storage medium and/or conducting binder in electrochemical batteries. Specifically, nano-sized graphite (which is also sometimes called “amorphous carbon”, as opposed to truly amorphous or “glassy” carbon) has been used as anode for Na ion batteries. Amorphous carbon as anode material has been investigated for Li insertion [3]. Glassy carbon in nanocomposites can be a component of electrodes. An increasing interest lies in the combination of different materials, composite materials, e.g. amorphous phosphorous/carbon composite and nanocomposite Sb/C were investigated as promising anode materials for Na-ion batteries.

We present a comparative ab initio computational study of sodium and lithium storage in amorphous (glassy) carbon (*a*-C) vs. graphite. Amorphous structures are obtained by fitting stochastically generated structures to a reference radial distribution function. Li insertion is thermodynamically favored in both graphite and *a*-C. While sodium insertion is thermodynamically unfavored in graphite, *a*-C possesses multiple insertion sites with binding energies stronger than Na cohesive energy, making it usable as anode material for Na ion batteries.



In the figure: (Left) Na insertion sites in a-C. (Right) The defect formation energies E_f of Li and Na with respect to bulk Li and Na, respectively, in a-C. The corresponding E_f values in graphite are also shown as black circles.

[1] F. Legrain, O. Malyi, S. Manzhos, Comput. Mater. Sci. 94, 214 (2014)

[2] S. C. Jung et al., J. Phys. Chem. Lett. 5, 1283 (2014)

[3] G. Gourdin, P.H. Smith, T. Jiang, T.N. Tran, D. Qu, J. Electroanalytical Chemistry 688, 103 (2013)