# Theoretical Study on Capacitance Origin of Modified Graphene Cathode in Lithium Ion Capacitor

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Graphene with different structure is used widely as cathode of lithium ion capacitor (LIC) [1-2]. However, the origin of capacitance behavior in the work voltage range of LIC is still not very clear [3-4]. In this article, the quantum capacitance and corresponding electronic origin of various graphene material are investigated by DFT method. It is found that the capacitance contribution of graphene based material are mostly from the π and the σ electron from unbonded atoms, depending on the type of graphene structure. Graphene with pentagon defects possess higher quantum capacitance than pristine one due to the contribution from the π electron located at the pentagon. The introduction of B can contribute to quantum capacitance, while N, P does not work. One atom defected graphene and pyrrolic N doped graphene demonstrates very high quantum capacitance due to the presence of unbonded σ electron. And pyridinic graphene shows even higher quantum capacitance due to the presence of unpaired electron from N atom. Although there are residual O in graphene, they have very seldom quantum capacitance effect in the voltage range of graphene cathode.

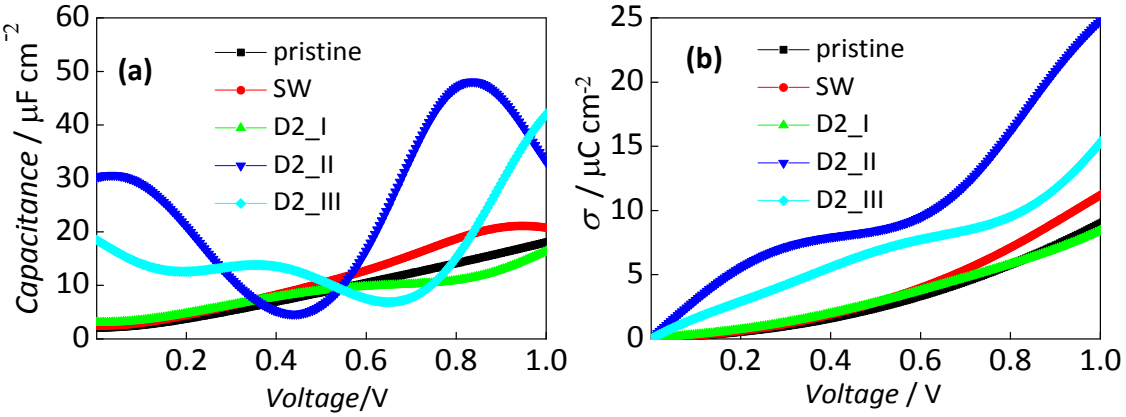


Figure 1. Quantum capacitance of pristine and graphene with SW and D2 defects. (a): quantum capacitance and (b) excessive surface charge density.

**References:**

[1] G. G. Amatucci, F. Badway, A. Du Pasquier, T. Zheng, Journal of The Electrochemical Society 2001, 148, A930-A939.
[2] B. C. Wood, T. Ogitsu, M. Otani, J. Biener, The Journal of Physical Chemistry C 2014, 118, 4-15.
[3] J. Vatamanu, X. Ni, F. Liu, D. Bedrov, Nanotechnology 2015, 26, 464001.
[4] C. Zhan, Y. Zhang, P. T. Cummings, D.-e. Jiang, Carbon 2017, 116, 278-285.