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# Supercapacitor electrodes based on Nanocarbon-Transition Metal Oxides/Chalcogenides Hybrids with Insight from Density Functional Theory Investigations

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## Abstract

The ever-growing global demand of energy together with the depletion of fossil fuels makes it critical to develop sustainable and renewable energy resources. Developing relevant energy storage systems such as supercapacitors and batteries is

essential to utilizing sustainable and renewable energy resources. Supercapacitors store energy in terms of both electrostatic double layer capacitance (EDLC) and pseudocapacitance. Nanostructured hybrid materials with both organic and inorganic components have attracted much attention recently due to the possibility of tailoring their dimensionality to facilitate a change in their fundamental properties including redox potential, conductivity and charge storage, in comparison with those of their bulk analogs. In my talk, I'll discuss the working principles and fundamental aspects of supercapacitors and the recent achievements of our research group on design of 2D layered materials and reduced graphene oxide hybrids for supercapacitor applications. Some of our recent findings on supercapacitors based on graphene analogue 2D layered materials, nanosheets and their hybrids for high performance supercapacitors will be highlighted. Also, the effect of nanostructures on the properties of supercapacitor performances including specific capacitance, rate capability, energy density, power density and cycle stability for the next generation of supercapacitor electrode design will be discussed.



#### **Biography:**

Chandra Sekhar Rout is an Assoc. Prof. at Jain University, Bangalore. He did his postdoctoral research at National University of Singapore (2008-2009), Purdue University, USA (2010-2012) and UNIST, South Korea (2012-2013). His current google scholar h-index is 30 with total citations ~5200. He is associate editor of "RSC Advances" a journal of Royal Society of Chemistry and "American Journal of Engineering and Applied Sciences" of Science Publications.

#### Speaker Publications:

1. "NHC-Pd complex heterogenized on graphene oxide for cross-coupling reactions and supercapacitor applications"; Applied Organometallic Chemistry; 2020.

2. "A comparative experimental and theoretical investigation on energy storage performance of CoSe2, NiSe2 and MnSe2 nanostructures"; Applied Materials Today; vol 19, 2020, 100568.

3. "Two-Dimensional Layered Metallic VSe 2 /SWCNTs/rGO Based Ternary Hybrid Materials for High Performance Energy Storage Applications"; Chemistry; vol 26, 2020.

4. "Partially graphitized Iron-carbon hybrid composite as electrochemical supercapacitor material"; ChemElectroChem; vol 07, 2020, 1928-1934.

5. "Comparative Electrochemical Energy Storage Performance of Cobalt Sulfide and Cobalt Oxide Nanosheets: Experiment & Theoretical Insight From Density Functional Theory Simulations"; Physical Chemistry Chemical Physics, vol 22, 2020.

<u>6th International Conference on Physical and Theoretical</u> <u>Chemistry</u>; Webinar; March 18 -19, 2020.

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