



## 65th DAE SOLID STATE PHYSICS SYMPOSIUM

Dec 15 - 19, 2021

# PROGRAMME & ABSTRACTS

Venue DAE Convention Centre Anushaktinagar, Mumbai

Organized by Bhabha Atomic Research Centre Mumbai



Sponsored by
Board of Research in Nuclear Sciences
Department of Atomic Energy
Government of India

### 65th DAE Solid State Physics Symposium

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## Programme and Abstracts









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Sakshi Kansal<sup>1</sup>, Paulomi Singh<sup>2</sup>, Debabrata Mandal<sup>2</sup>, Vikas Sharma<sup>2</sup>, Trilok Singh<sup>1</sup> and

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Cr<sub>2</sub>O<sub>3</sub> is considered to be a promising cathodic material for supercapacitor applications on the promising cathodic material for supercapacitor applications on the account of its fast redox kinetics, mesoporous structure, and better electrochemical stability. Herein, we introduced a one-step synthesis of Cr2Os which depicts a unique cactuslike morphology. Such structure improves the specific surface area and ion diffusion mechanism, which enhances the capacitance value. The prepared Cr<sub>2</sub>O<sub>1</sub> displayed a specific capacitance value of 35 F g<sup>-1</sup> at 5 mV s<sup>-1</sup>, with capacitive retention of  $\sim 60\%$  at a scan rate as bigh as 150 graph at 5 mV s<sup>-1</sup>, with capacitive retention of  $\sim 60\%$  at a scan rate as high as 150 mV s<sup>-1</sup>. This can be attributed to the redox couple of Cr<sup>4+</sup>/ Cr<sup>3+</sup> displayed by Ct2O3 at the electrode-electrolyte interface. Hence, cathodic electrodes based on such novel morphology of Cr<sub>2</sub>O<sub>3</sub> can be used for devising high-performance supercapacitors, with appreciable chemical stability, and rate performance

### 10080

High Performance Na-ion Supercapacitor: Beyond Carbon Structures

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Recent trends in sodium-ion-based energy storage devices have shown a potential use of hollow structures as an electrode material to improve the performance of storage systems. Carbon based material are also the leading material with sodium-based electrode materials. In this paper, V<sub>2</sub>O<sub>5</sub> nanorods have been employed as the efficient electrode material for Naion batteries. These nanostructures showed impressive electrochemical activity in 2 M NaOH electrolyte owing to their redox activity.

Role of Minority-spin States and Cu Doping on CO Interaction over Pt<sub>3</sub>Cu Nanocluster Hemang P. Tanna<sup>1, \*</sup>, Bhumi A. Baraiya<sup>1</sup> and Prafulla K. Jha<sup>1</sup>

Department of Physics, Faculty of Science, The M. S. University of Baroda, Vadodara,

First-principles based on dispersion corrected spin-polarized density functional theory (DFT-D3) calculations were performed to investigate the structural properties, relative energetics, and electronic reactivity descriptors (ERDs) of neutral and charged Pt4, Cu4, and Pt5Cu NCs. The interaction mechanism of CO over energetically preferable NCs was examined and our results of ERDs indicate that the doping of Cu atom reduces the strength of CO on Pt atom which can eliminate the poisoning effect of CO.

Evaluation of Xanthan gum with additive salts as an electrolyte for Sodium-ion.

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The skyrocketing demand of Lithium ion batteries (LIBs) leads to the urge to develop The skylocketing demand of Lithium for batteries (LIBs) leads to the arge to develop potential energy storage devices. Sodium-ion batteries (SIBs) could be a good alternative due