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Original Article

ICOD-SC: Internal Carbon Optimized Distribution for Next-Generation Supercapacitors - A Carbodome-Inspired Framework for Rational Design of Carbon-Based Energy Storage

Devprakash R¹, Rajasekaran E²

¹School of AI Computing & Multimedia, Lincoln University College, Petaling Jaya, 47301, Malaysia.

²Carbonix-Theta, India.

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ABSTRACT

Supercapacitors offer rapid charge-discharge, high power density and long cycle life, with carbon-based electrodes providing high conductivity, stability, porosity and surface area. However, practical performance depends not only on nominal surface area but also on carbon accessibility, pore architecture, ion transport, conductivity, surface chemistry and electrolyte properties. This article proposes **ICOD-SC (Internal Carbon Optimized Distribution for Supercapacitors)**, a conceptual framework inspired by carbon-distribution concepts in proteins. Two new research descriptors, **Cfrac-SC** and **Carbodome-SC**, are proposed to quantify accessible carbon and the combined effects of carbon accessibility, pore structure, ion transport, conductivity and surface functionality. Experimental validation using controlled carbon architectures and full-cell electrochemical testing is required to establish their predictive value.

KEYWORDS

Supercapacitor, Carbon Electrode, Carbon Distribution, ICOD-SC, Carbodome-SC, Cfrac-SC, Porous Carbon, Hierarchical Porosity, Ion Transport, Electrochemical Energy Storage.

1. INTRODUCTION

The transition toward renewable energy, electrified transportation and distributed energy systems has increased the need for energy-storage technologies capable of rapid charge and discharge while maintaining long operational lifetimes (Devprakash et al., 2025; Rajasekaran, Meenal, et al., 2024; Simon & Gogotsi, 2008).

Two principal mechanisms contribute to supercapacitor charge storage. In an electric double-layer capacitor (EDLC), charge is stored predominantly through electrostatic adsorption of electrolyte ions at the electrode/electrolyte interface. In pseudocapacitive systems, fast and reversible surface or near-surface redox processes additionally contribute to charge storage (Simon & Gogotsi, 2008).

Porous carbon is particularly important for EDLC electrodes because it can combine electrical conductivity, chemical stability and tunable pore structures. The electrochemical usefulness of a porous carbon electrode, however, depends on more than its nominal structural surface area. Electrolyte access to the relevant pores, pore connectivity, ion transport, electronic conduction and surface chemistry can determine how much of the available carbon participates effectively in charging (Borchardt et al., 2018; Conway, 1999; Huang et al., 2017; Idris et al., 2026; Liu et al., 2017; Wang et al., 2025).

The present work therefore asks a materials-design question: can the spatial organization of carbon within a porous electrode be treated as an explicit design variable and linked quantitatively to electrochemical function? ICOD-SC is proposed as a framework for testing this question. It does not replace established electrochemical double-layer theory or conventional structural characterization. Instead, it organizes structural and electrochemical information into a testable structure–distribution–function hypothesis.

2. FROM CARBON DISTRIBUTION IN PROTEINS TO CARBON DISTRIBUTION IN MATERIALS

The conceptual origin of ICOD-SC lies in carbon-distribution analysis developed for protein sequences and structures. CARBANA treated carbon content and distribution as descriptors associated with hydrophobic/hydrophilic characteristics (Rajasekaran & Vijayasathy, 2011). CARD extended the analysis to carbon distribution at residue resolution (Rajasekaran, 2012), and CARD-3D extended the concept to three-dimensional structural organization (Rajasekaran et al., 2014). The Carbodome concept subsequently proposed a relationship between carbon distribution and protein stability and function ((Indupriya & Rajasekaran, 2024; Rajasekaran, 2025).

The present materials-science extension is conceptual:

Carbon composition → carbon distribution → functional domains

For proteins, the functional outcome may involve folding, stability and molecular interactions, including relationships between carbon distribution and functional behaviour

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(Indupriya & Rajasekaran, 2024; Rajasekaran, Devprakash, et al., 2024; Rajasekaran, 2025). For porous carbon electrodes, the corresponding outcome may involve electrolyte access, ion transport, electronic conduction and charge storage. These systems involve fundamentally different physical mechanisms; therefore, the analogy is a framework for organizing a design hypothesis rather than evidence of a shared mechanism.

3. ICOD-SC HYPOTHESIS

The central hypothesis is that a porous carbon electrode may possess an optimum internal organization of carbon and pores that maximizes useful electrochemical accessibility while maintaining efficient ion transport, electronic conductivity and structural integrity. The hypothesis does not imply that carbon atoms themselves simply attract electrolyte ions because of their presence. Relevant physical variables include carbon surface area, pore dimensions, pore connectivity, accessibility, surface functional groups, electronic conductivity, electrolyte composition, ion solvation/desolvation, electrode thickness and carbon packing density (Borchardt et al., 2018; Conway, 1999; Huang et al., 2017; Idris et al., 2026; Liu et al., 2017; Simon & Gogotsi, 2008; Wang et al., 2025). ICOD-SC therefore treats carbon organization as one component of a coupled electrode architecture. The experimental test is whether controlled differences in this organization produce reproducible changes in electrochemical behaviour after major formulation and cell-level confounders have been controlled.

4. CARBON DISTRIBUTION VERSUS PORE-SIZE DISTRIBUTION AND CONNECTIVITY

Carbon distribution and conventional pore-size distribution/connectivity are related but distinct. Pore-size distribution describes the geometry of the void space: pore dimensions, pore-volume contributions and, where measurable, the connectivity or hierarchy of the pore network. Gas adsorption and NLDFT analysis provide conventional routes for characterizing these properties. Carbon distribution, as used here, refers to the spatial organization of the carbon-containing solid phase and its functional environments within the electrode.

The proposed architecture distinguishes, for example, a conductive carbon backbone, mesoporous transport regions, microporous charge-storage regions and surface-functional carbon domains. Thus, pore structure describes the complementary void space, whereas carbon distribution describes organization of the solid carbon phase and its functional domains. The two quantities are coupled but are not interchangeable. Two electrodes may have comparable pore-size distributions while differing in the organization of conductive carbon pathways or functional domains; conversely, similar carbon compositions may be associated with different pore architectures. In Carbodome-SC, pore architecture is therefore retained as a separate component rather than used as a surrogate for carbon distribution.

5. PROPOSED ICOD-SC ELECTRODE ARCHITECTURE

A first-generation ICOD-SC electrode can be represented by four principal carbon environments:

- Conductive carbon backbone: a continuous network intended to provide low-resistance electron transport. Candidate materials include graphitized carbon, reduced graphene oxide, carbon nanotubes and carbon nanofibres.
- Mesoporous transport region: mesopores can facilitate electrolyte penetration and transport toward smaller pores.
- Microporous charge-storage region: micropores can provide substantial interfacial area for electric-double-layer formation; optimum dimensions depend on electrolyte-ion size and solvation behaviour.
- Surface-functional carbon: controlled nitrogen, oxygen, sulfur, phosphorus or other functionality can modify wettability, electronic properties and pseudocapacitive contributions (Huang et al., 2017; Wang et al., 2025).

The design objective is therefore not simply maximum carbon or maximum nominal surface area, but coordinated organization of conductive, transport, charge-storage and functional domains.

6. ELECTROCHEMICAL BASIS

For an idealized capacitor, stored energy is:

$$E = 1/2 CV^2$$

where E is stored energy, C is capacitance and V is operating voltage. At an electrochemical interface, capacitance depends on the effective interfacial area and charge-separation characteristics. A simplified relation is:

$$C \propto \epsilon A/d$$

where ϵ is an effective dielectric permittivity, A is electrochemically accessible interfacial area and d represents an effective charge-separation distance. In ICOD-SC, A is not assumed to be identical to the total nominal internal area. The framework instead proposes measuring accessibility through a combined structural-electrochemical procedure.

7. PROPOSED CFRAC-SC DESCRIPTOR

Cfrac-SC is proposed as an operational descriptor of the fraction of the carbon phase that is electrochemically accessible under defined electrolyte and charging conditions:

$$C_{\text{frac-SC}} = \text{electrochemically accessible carbon} / \text{total carbon}$$

At the present conceptual stage, electrochemically accessible carbon cannot be obtained by simply counting carbon atoms exposed to the atmosphere. It must be operationally defined under specified electrochemical conditions.

7.1. Operational Determination of Electrochemically Accessible Carbon

The proposed determination will use a two-stage procedure. First, the structural carbon inventory and pore environment will be characterized using carbon mass, BET/gas adsorption and NLDFT pore-size distribution, together with microscopy where appropriate. These measurements establish the total carbon loading and the structural population of potentially accessible pores. Second, electrochemical utilization will be quantified using a standardized electrolyte, cyclic voltammetry, galvanostatic charge-discharge and electrochemical impedance spectroscopy. The electrochemical response will identify the fraction of the structurally available carbon/pore environment that contributes measurably and reversibly under the defined charging protocol. A calibrated operational accessibility factor will then be assigned to the structurally accessible carbon population. The resulting Cfrac-SC will be reported together with the electrolyte, voltage window, current density and structural measurement conditions.

Because the mapping between electrochemical capacitance and carbon mass is not universal, the manuscript does not claim that Cfrac-SC can be obtained from BET area alone. Instead, the proposed protocol explicitly combines structural and electrochemical measurements. A reproducible calibration procedure will be established during experimental validation, and uncertainty in Cfrac-SC will be reported.

Cfrac-SC is a proposed descriptor and has not yet been experimentally validated.

8. PROPOSED CARBODOME-SC INDEX

Carbodome-SC is proposed as a dimensionless composite descriptor:

$$\text{Carbodome-SC} = w_1CA + w_2P + w_3I + w_4E + w_5F$$

where CA is normalized carbon accessibility, P is normalized pore-architecture quality, I is normalized ion-accessibility/transport, E is normalized electronic-conductivity performance and F is normalized surface-functionality performance. The weights w_1 – w_5 are parameters to be determined experimentally.

8.1. Normalization of CA, P, I, E and F

Because the five components have different units and ranges, each will first be transformed to a dimensionless 0–1 score. For a beneficial variable, min-max normalization will be used:

$$X_{\text{norm}} = (X - X_{\text{min}})/(X_{\text{max}} - X_{\text{min}})$$

For a variable for which lower values indicate better performance, inverse normalization will be used:

$$X_{\text{norm}} = (X_{\text{max}} - X)/(X_{\text{max}} - X_{\text{min}})$$

The definitions of X_{min} and X_{max} will be fixed from the predefined experimental dataset or a physically justified calibration range and will not be changed between samples after the analysis has begun. This prevents selective rescaling of individual electrodes.

CA will represent Cfrac-SC on the normalized 0-1 scale. P will be constructed from predefined pore-size-distribution and connectivity measures. I will be derived from standardized ion-transport/accessibility indicators obtained principally from EIS and rate-dependent electrochemical response. E will be based on electronic conductivity/resistance measurements. F will be derived from surface-chemical measurements, principally XPS and elemental analysis, supplemented by wettability and electrochemical evidence where appropriate.

8.2. Determination of Weighting Factors

The weighting factors will not be assigned solely from qualitative judgement. Equal weights ($w_i = 0.20$) may be used as an initial baseline for exploratory analysis. Final weights will be estimated from the experimentally measured dataset using constrained multivariable modelling, with non-negative coefficients and a unit-sum constraint:

$$w_i \geq 0; \quad \sum w_i = 1$$

The response variables will include specific capacitance, ESR, rate-capability retention and cycle retention. Cross-validation will be used to reduce overfitting, and the final weights will be tested against independent electrode samples. Sensitivity analysis will be used to determine whether moderate changes in the weights materially alter the ranking of electrode architectures.

The purpose is to test whether the composite descriptor provides predictive information beyond individual conventional descriptors, particularly BET surface area. Carbodome-SC is therefore a proposed research descriptor and has not yet been experimentally validated.

9. WHY NOMINAL SURFACE AREA ALONE IS INSUFFICIENT

BET surface area remains an important conventional structural descriptor and will be measured in the proposed experimental programme. The specific issue addressed by ICOD-SC is that nominal internal area does not necessarily equal the area effectively utilized under a particular electrolyte and charging rate. Pore accessibility, ion transport, electronic resistance, surface chemistry and electrode density can modify practical performance (Borchardt et al., 2018; Huang et al., 2017; Liu et al., 2017; Wang et al., 2025).

Accordingly, the framework does not reject high surface area. Rather, it asks whether a combination of accessibility and functional organization can explain differences between electrodes that cannot be explained by BET area alone. The experimental comparison will test this proposition rather than assume it.

10. SURFACE CHEMISTRY AND FUNCTIONAL CARBON

Heteroatom incorporation can modify wettability, electronic structure, active sites, redox behaviour and pseudocapacitive contributions (Huang et al., 2017; Wang et al., 2025). Such functionality may therefore alter the electrochemical environment of the carbon phase. ICOD-SC treats heteroatoms as modifiers of the carbon environment rather than simply as additives.

The target is controlled surface chemistry without excessive defects or loss of conductivity. Surface functionality will be characterized using XPS and elemental analysis, with electrochemical measurements used to determine whether the chemical modification produces measurable changes in wettability or charge-storage behaviour.

11. PROPOSED MATERIALS STRATEGY

- Graphitized carbon/CNT/rGO as an electron-conduction backbone.
- Mesoporous carbon as an ion-transport component.
- Activated microporous carbon as a principal EDLC surface.
- Controlled N/O/S/P functionality for wettability and possible pseudocapacitive contribution.
- A common conductive binder system and common current collector across the comparative electrode series.

The exact composition will be determined experimentally. The proposed components define a design space rather than a claimed optimal formulation.

12. PROPOSED FABRICATION STRATEGY

- Stage 1 – Construct a continuous conductive carbon network.
- Stage 2 – Introduce controlled mesoporosity using established pore-engineering methods.
- Stage 3 – Generate micropores capable of providing high electrochemical interfacial area.
- Stage 4 – Introduce controlled surface functionality while limiting detrimental loss of conductivity or structural integrity.
- Stage 5 – Characterize and, where feasible, control electrode packing density because porosity can influence both gravimetric and volumetric performance.

All comparative electrodes will undergo the same mixing, coating, drying, pressing and conditioning procedures except where a procedure is intentionally changed to create the target architecture.

13. EXPERIMENTAL VALIDATION AND CONTROLS

The central validation experiment will compare carbon electrodes with controlled differences in carbon/pore architecture. The proposed series is:

- SC1 – micropore-dominant.

- SC2 – mesopore-dominant.
- SC3 – hierarchical micro/mesoporous.
- SC4 – hierarchical architecture with a conductive carbon network.
- SC5 – hierarchical architecture with optimized surface chemistry.

The interpretation of these comparisons requires control of variables unrelated to the intended architecture. Total active-material composition, active-material mass loading, binder type and ratio, current collector, electrode area, electrolyte, cell configuration and electrochemical testing conditions will be kept constant. Thickness and dry density will be measured for every electrode. Exact matching of thickness or density may not always be physically possible because pore architecture itself affects packing; therefore, residual differences will be reported and included as covariates or controlled variables in the analysis.

Structural characterization will include SEM, TEM, BET/gas adsorption, NLDFT pore-size distribution, Raman spectroscopy, XPS and elemental analysis. Electrochemical characterization will include cyclic voltammetry, galvanostatic charge-discharge, electrochemical impedance spectroscopy, leakage/self-discharge measurements, cycling stability and rate capability.

13.1. Electrochemical Performance Calculations

Two-electrode full-cell testing will be the primary basis for comparing practical device performance. For a symmetric cell, specific capacitance will be calculated from the galvanostatic discharge curve:

$$C_{sp} = I\Delta t / (m\Delta V)$$

Where I is discharge current, Δt is discharge time, ΔV is the effective discharge voltage after accounting for the initial IR drop, and m is the total active carbon mass in the two electrodes. The mass convention will be stated explicitly and applied consistently.

ESR will be estimated from the instantaneous voltage drop at the start of discharge:

$$ESR = \Delta V_{IR} / I$$

ESR will also be assessed using EIS as an independent electrochemical measurement. Rate capability will be reported as capacitance retention at progressively increasing current densities relative to a defined reference current density:

$$Rate\ retention\ (\%) = 100 \times C_{sp,high-current} / C_{sp,reference}$$

Cycle retention will be reported as:

$$Cycle\ retention\ (\%) = 100 \times C_N / C_1$$

where C_1 is the capacitance of the first cycle and C_N is the capacitance after N cycles. Current density, voltage window, temperature, mass loading, cell configuration and cycle number will be reported with each result. Coulombic efficiency will also be monitored where appropriate.

Two-electrode full-cell data will be distinguished from any three-electrode electrode-level measurements. This is intended to prevent overinterpretation of three-electrode performance as a direct measure of practical device behaviour (Idris et al., 2026).

14. PROPOSED CORRELATION AND STATISTICAL ANALYSIS

The principal test will examine relationships between Carbodome-SC and specific capacitance. Secondary analyses will examine Carbodome-SC against ESR, rate-capability retention and cycle retention. Cfrac-SC will be tested separately against the same response variables.

Correlation will not be interpreted as proof of causation. Multivariable modelling will be used to determine whether the composite descriptor retains predictive value after accounting for conventional structural variables such as BET area, pore volume, density and mass loading. Cross-validation and, where possible, independent validation electrodes will be used to assess generalization.

The expected relationship need not be linear. At low optimization, insufficient accessible carbon or poor ion transport may dominate; at an intermediate architecture, accessibility, transport and conductivity may be balanced; excessive porosity or poor packing may reduce volumetric performance or increase resistance. These are hypotheses to be tested, not established outcomes.

15. EXPERIMENTAL CONTROLS AND CONFOUNDING VARIABLES

Table 1: Controlled Variables and Reporting Strategies for Comparative Electrode Evaluation

Variable	Control/reporting strategy
Total carbon / active-material composition	Matched as closely as practicable; exact composition reported.
Mass loading	Matched across comparative electrodes; reported as mg cm^{-2} .
Thickness	Measured after fabrication and reported; differences included in analysis.
Dry density	Calculated from mass and volume; reported and treated as a controlled variable.
Binder	Same binder chemistry and binder-to-active-material ratio.
Current collector	Same material, geometry, pretreatment and contact procedure.
Electrolyte	Same electrolyte composition, concentration and conditioning protocol.
Cell configuration	Same two-electrode full-cell geometry and electrode spacing.
Testing conditions	Same voltage window, temperature, current-density/scan-rate protocol.

16. ENERGY AND POWER CONSIDERATIONS

For a capacitor, stored energy follows $E = 1/2 CV^2$. Thus, increasing capacitance is one route to higher energy, while increasing the safe voltage window has a squared effect. ICOD-SC therefore does not treat carbon architecture independently of electrolyte and operating voltage. Ion size, solvation, pore confinement and electrolyte stability can influence which regions of the pore network are effectively utilized (Borchardt et al., 2018; Simon & Gogotsi, 2008).

17. CARBON DISTRIBUTION-ENERGY STORAGE RELATIONSHIP

Carbon distribution → functional carbon domains → ion/electron organization → electrochemical function

This proposed progression parallels the conceptual structure of earlier carbon-distribution studies in proteins, but it is not a mechanistic equivalence. The materials-science hypothesis is that spatial organization of the carbon phase, together with the pore network and surface chemistry, may provide a useful structure–function descriptor for energy storage.

18. PROPOSED NAME AND INTELLECTUAL FRAMEWORK

The proposed technology is designated ICOD-SC (Internal Carbon Optimized Distribution for Supercapacitors), with Carbodome-SC denoting the broader carbon-domain descriptor framework for electrochemical energy storage.

- Central Design Philosophy: “Optimize where the carbon is, not merely how much carbon is present.”
- Scientific Formulation: “The electrochemical performance of porous carbon electrodes may be influenced by the spatial distribution, accessibility and functional organization of carbon within the electrode, in addition to conventional descriptors such as total carbon content and nominal surface area.”

19. LIMITATIONS AND FALSIFIABILITY

Cfrac-SC and Carbodome-SC are proposed descriptors and have not yet been experimentally validated. Their definitions, normalization ranges, weighting factors and predictive value must therefore be established through systematic experiments. Carbon distribution cannot be considered independently of pore structure, electrolyte chemistry, electrode density and electrode construction. BET surface area remains an important descriptor. The proposed framework must demonstrate predictive value beyond conventional measurements rather than assume that it does.

The carbon-distribution analogy with proteins is conceptual and does not establish a common physical mechanism. The framework can be falsified if controlled variations in carbon organization fail to produce reproducible relationships with electrochemical accessibility or if Carbodome-SC provides no predictive improvement over conventional descriptors after appropriate controls. A further limitation is that electrochemically accessible carbon is an operational quantity rather than a directly observable count of carbon atoms. Its reproducibility will therefore depend on a standardized electrolyte, electrochemical protocol and calibration procedure. This limitation is explicitly recognized in the proposed validation strategy.

20. CONCLUSION

This revised manuscript proposes ICOD-SC as a conceptual framework for investigating carbon distribution as an explicit design variable in porous-carbon supercapacitor electrodes. The framework distinguishes carbon distribution from conventional pore-size distribution and

connectivity and combines both with carbon accessibility, ion transport, electronic conductivity and surface chemistry. -SC and Carbodome-SC are explicitly proposed, unvalidated descriptors.

Cfrac-SC will be operationalized using combined structural and electrochemical measurements, while Carbodome-SC will use normalized components and experimentally determined weights. SC1-SC5 will be compared under controlled formulation and two-electrode full-cell conditions, with mass loading, thickness, density, binder, current collector and electrolyte recorded and controlled. The central experimental question remains whether optimized carbon organization can predict electrochemical performance beyond conventional structural descriptors such as BET surface area. Only systematic experimental validation can establish whether the proposed descriptors are useful, redundant or falsifiable.

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