# Heteroatom-enriched polybenzoxazine as precursor for N, O co-doped carbon structures for supercapacitor application

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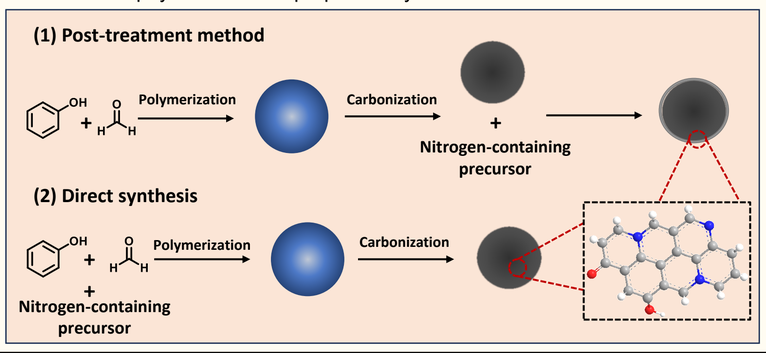
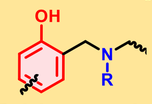
## INTRODUCTION

**Functionalized carbon structures**

- Low specific weight, tunable textural properties, ease of synthesis with cost feasibility
- CVD, Arc Discharge, Biomass pyrolysis: Demanding experimental conditions with formation of non-uniform polydisperse particles
- Carbonization of polymeric precursors: diverse synthesis routes, tailored molecular architecture and versatile chemical compositions
- Enhancement of physicochemical properties by introduction of heteroatoms



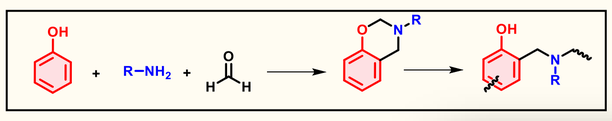

- ❑ Molecular design flexibility
- ❑ Inherent heteroatom doping
- ❑ High char yield
- ❑ High crosslinking density
- ❑ High dimensional stability
- ❑ Low volume shrinkage



**Polybenzoxazine**

**Direct heteroatom doping strategy to achieve bulk doping for tunable physicochemical properties**

## OBJECTIVE OF THE STUDY



**Conventional synthesis strategy**

**(1) Benzoxazine monomer synthesis**

**(2) Thermally accelerated ring-opening polymerization**

### One-step colloidal approach

Synthesis of polybenzoxazine colloidal particles using the modified sol-gel method

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Heteroatom-doped carbon via post-thermal treatment and controlled carbonization under inert conditions

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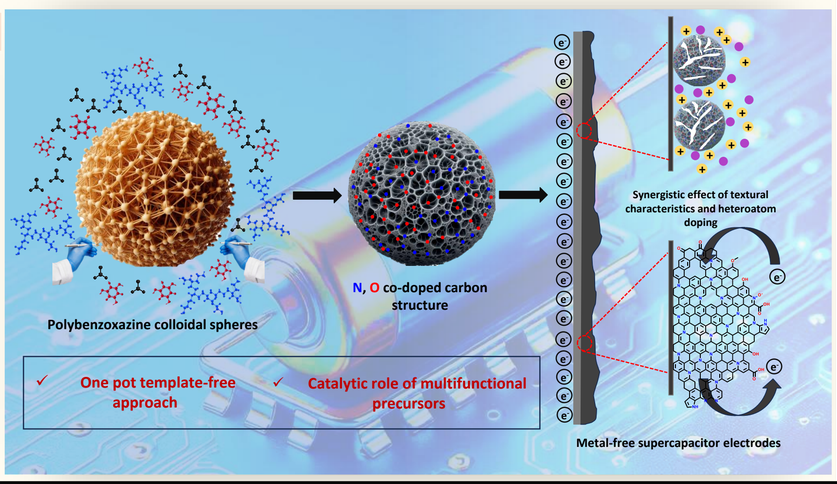
Utilization as active material for supercapacitor electrodes



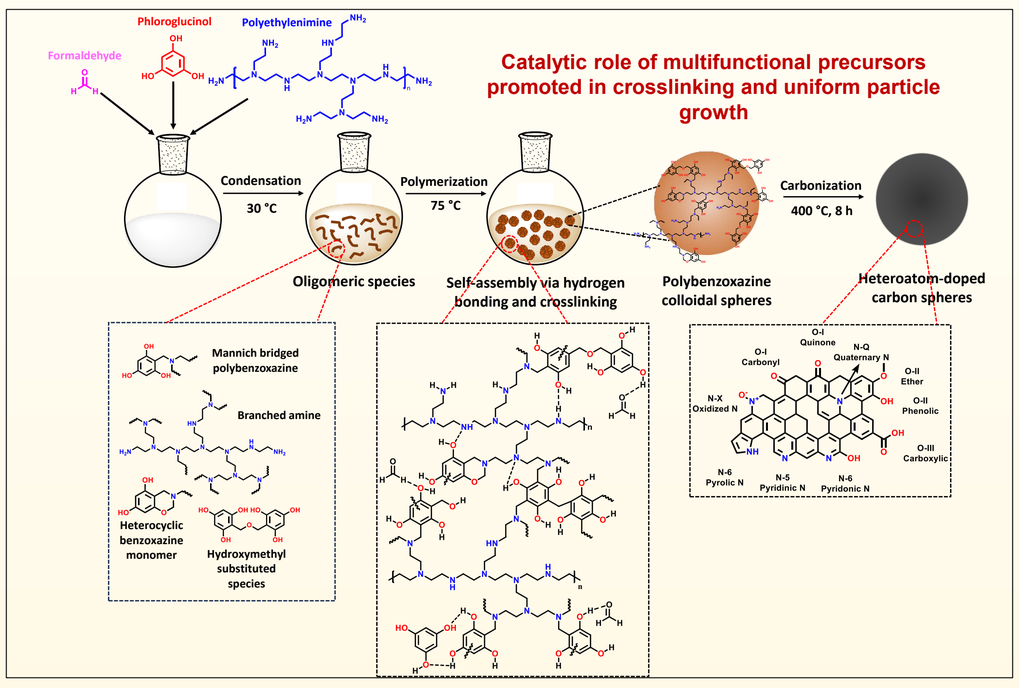

## SYNTHESIS OF POLYBENZOXAZINE PARTICLES

**Polymerization induced self-assembly influenced by**

**(1) Stoichiometric ratio of phloroglucinol: PEI: formaldehyde**

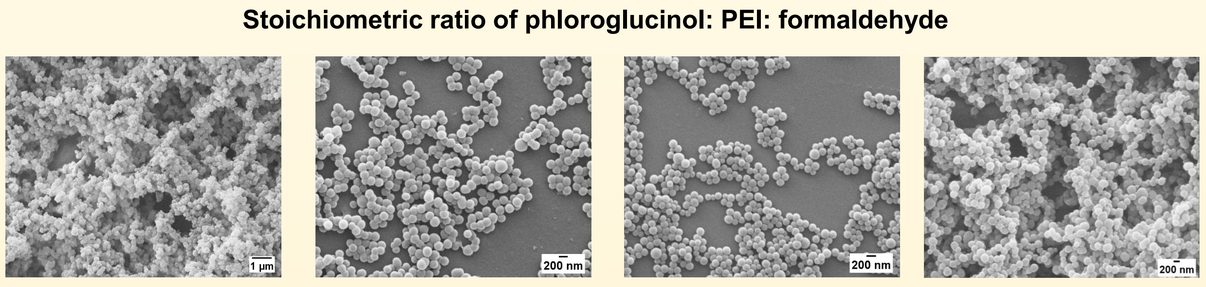
**(2) Ethanol/ water reaction medium ratio**

**(3) Precursor concentration**

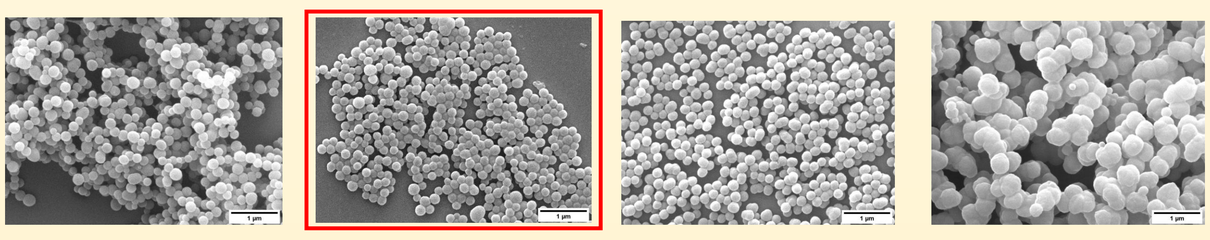



## OPTIMIZATION OF SYNTHESIS PARAMETERS

### Stoichiometric ratio of phloroglucinol: PEI: formaldehyde




### Ethanol/ water ratio



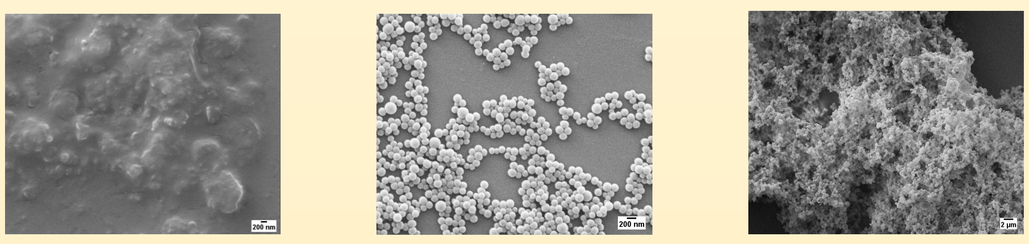
Ethanol/water: 0 %
Avg. Particle size ~ 197 ± 45 nm

Ethanol/water: 25%
Avg. Particle size ~ 160 ± 16 nm

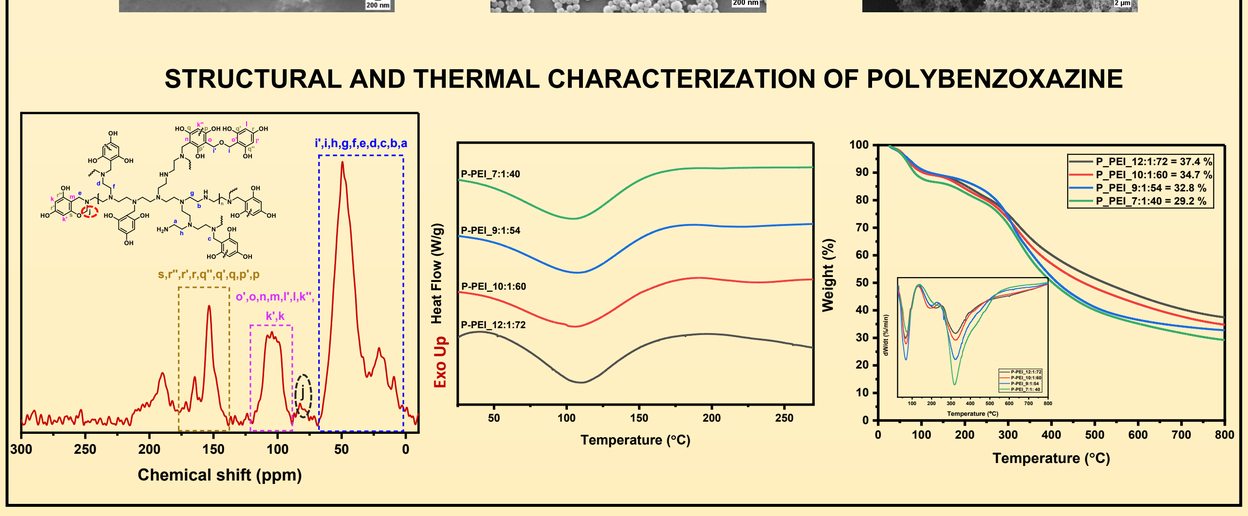
Ethanol/water: 75 %
Avg. Particle size ~ 224 ± 30 nm

Ethanol/water: 100 %
Avg. Particle size ~ 407 ± 64 nm

### Precursor concentration

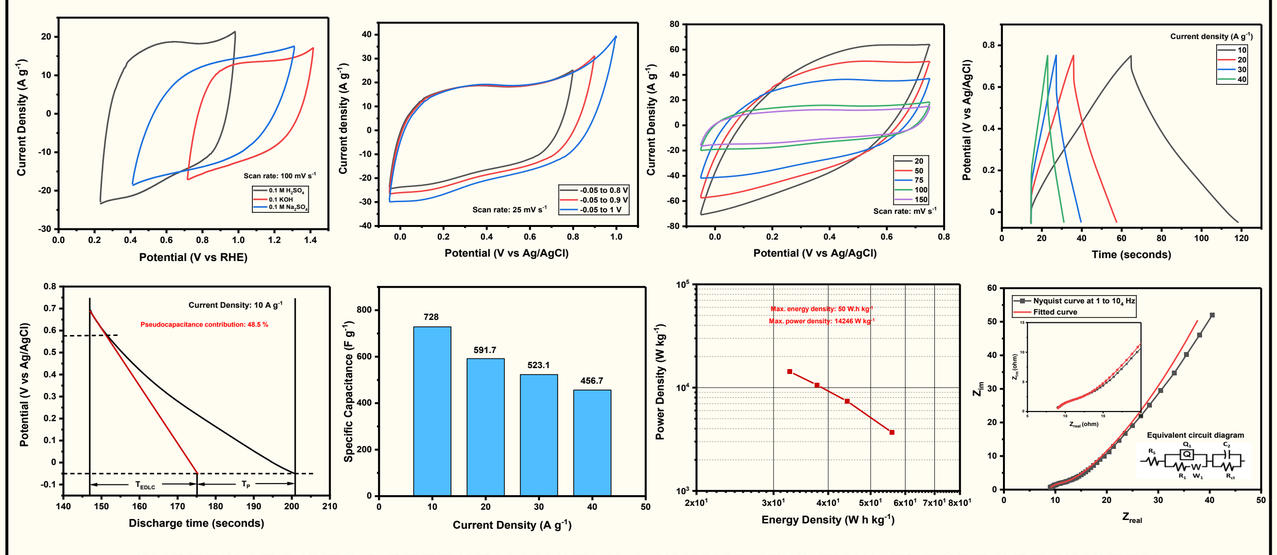



### STRUCTURAL AND THERMAL CHARACTERIZATION OF POLYBENZOXAZINE

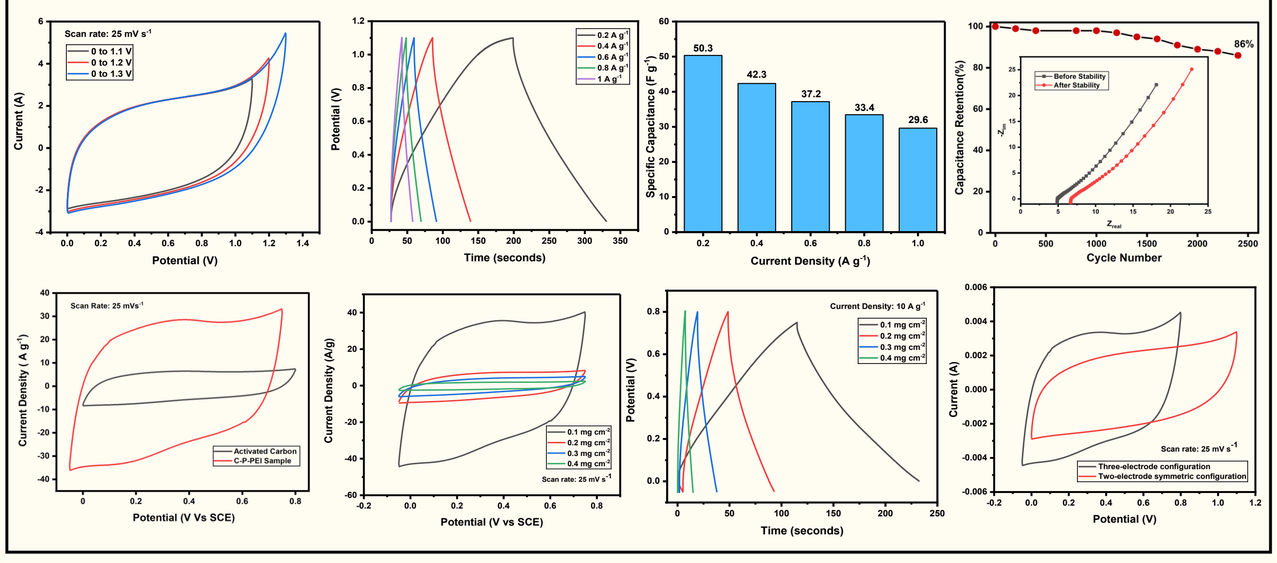



## SUPERCAPACITOR APPLICATION STUDIES

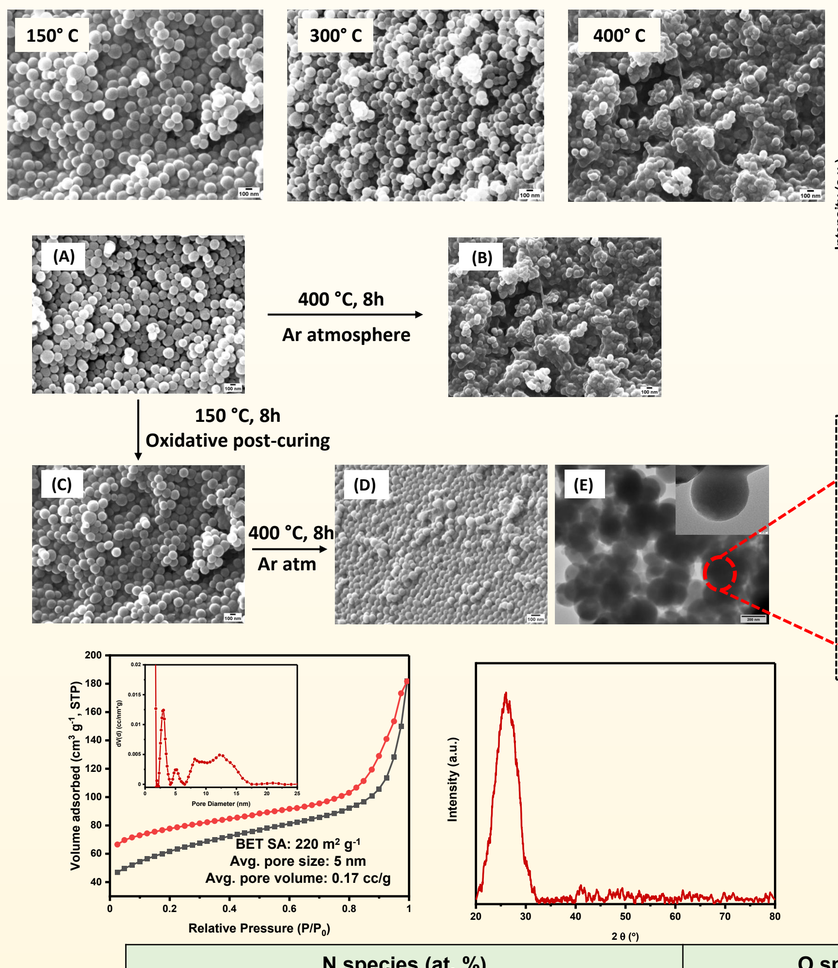
### SUPERCAPACITOR PERFORMANCE IN A THREE-ELECTRODE SYSTEM




### SUPERCAPACITOR PERFORMANCE IN A SYMMETRIC TWO-ELECTRODE SYSTEM




## CARBONIZATION FOR N,O-CODOPED CARBON

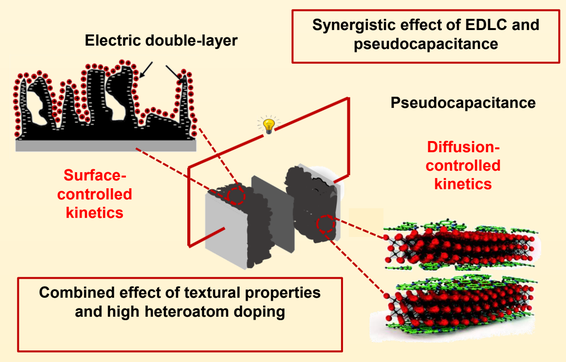


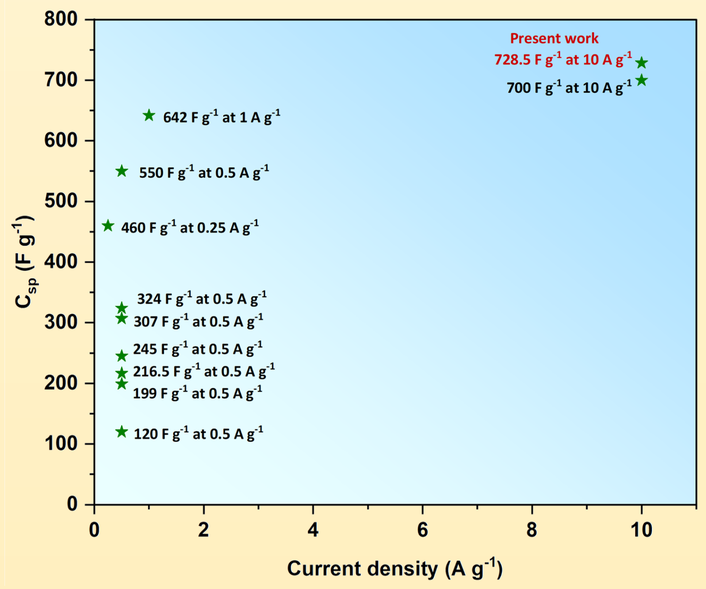

| C-P-PEI | % heteroatoms | |
|---|---|---|
| | XPS | CHNS |
| % C | 68.5 | 49 |
| % O | 10.92 | 20.5 |
| % N | 20.6 | 28.4 |

| N species (at. %) | | | | O species (at. %) | | |
|---|---|---|---|---|---|---|
| N-6 (396.3 eV) | N-5 (397.8 eV) | N-Q (398.8 eV) | N-X (402.7 eV) | O-I (529.4 eV) | O-II (531.3 eV) | O-III (532.1 eV) |

## CONCLUSION

- Polybenzoxazine as a potential source of heteroatom-doped carbon material by utilization of one-pot extended sol-gel process
- Process control by tuning of the stoichiometric ratio and the solvent system
- Catalytic role of multifunctional precursors
- Moderate carbonization conditions resulted in higher heteroatom doping and micro-mesoporosity
- Promising electrochemical performance in three- and two-electrode systems




**Comparative values of supercapacitor performance of C–P–PEI with literature reports of other polybenzoxazine-derived carbon materials**

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3 P. Sharma, V. Tanwar, **I. Tiwari,** P. P. Ingole and L. Nebhani, *Energy and Fuels*, 2023, **37**, 7445–7467.

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