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Python-Based Automated Response Surface Methodology: Computational Replication and Validation Framework for Supercapattery Materials Optimization

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INTRODUCTION & AIM

This study presents a complete computational framework for replicating, validating, and extending RSM-based optimization of $NiCo_2S_4$–graphene supercapattery materials through automated Python implementation, demonstrating the feasibility of reproducible computational design methodologies. RSM combined with CCD represents a powerful statistical approach for materials optimization in energy storage systems [1,2]. We replicated the optimization study [1] using a 20-experiment CCD with a five-level three-factor design.

Reproducibility & Transparency

Experimental Domain (Precursor Ratios, Time, Temp) → Input Data → Python Automation Framework (RSM Logic, ANOVA, Optimization) → Parameters → Optimized Material (Maximized Specific Capacitance)

Validation Loop

METHOD & RESULTS

Input: Design Matrix (CCD, 20 Runs)

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Variable Coding

$$x_i = \frac{X_i - X_{cp}}{\Delta X}$$

Experimental Domain (CCD Levels):

Factor	Low (-1)	Center (0)	High (+1)
X_1: G/NCS (%)	2.0	4.0	6.0
X_2: Time (h)	6.0	8.0	10.0
X_3: S/Ni Ratio	4.0	5.0	6.0

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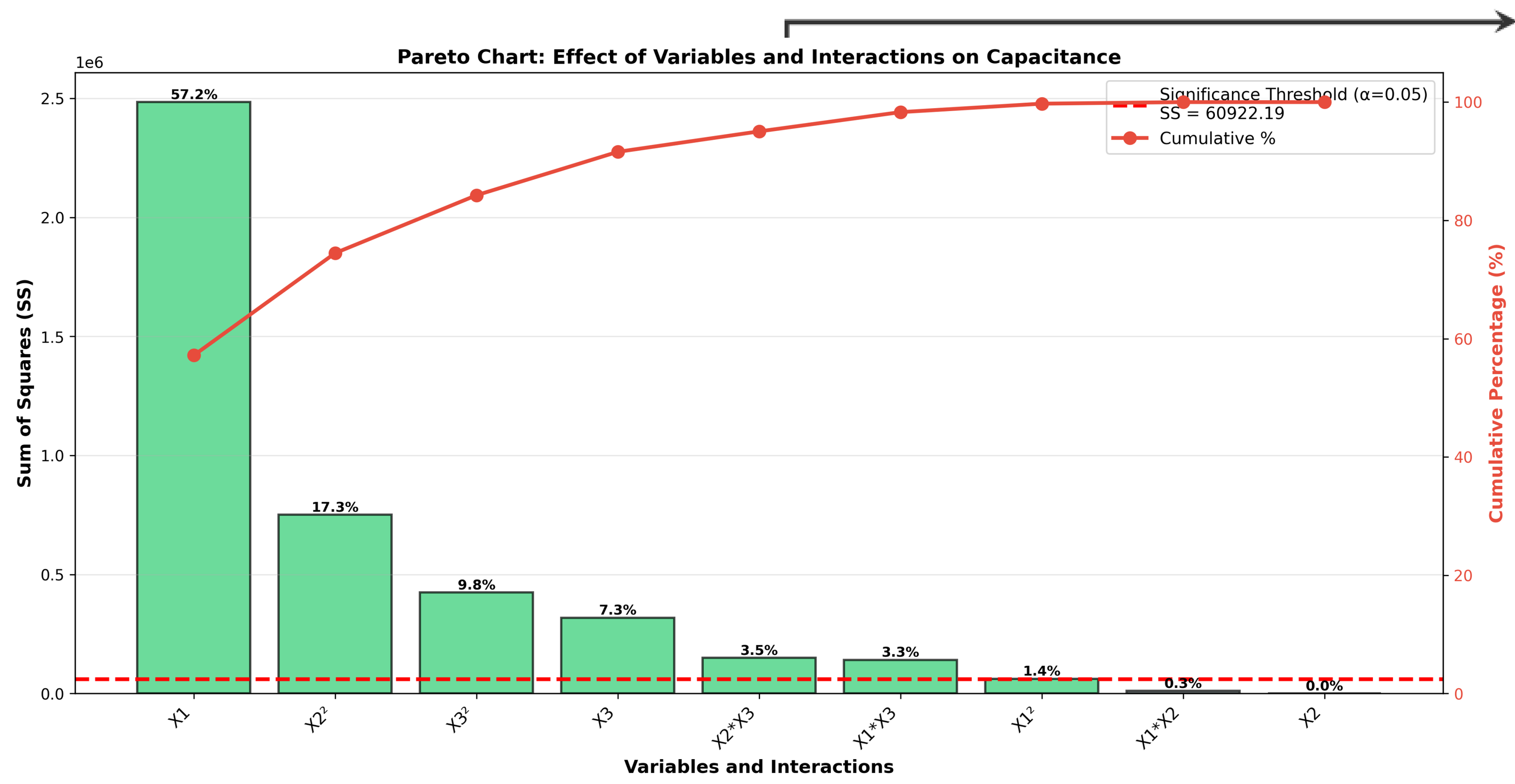
OLS Regression (Quadratic Model)

Fitted Polynomial Model (Y = Capacitance):

$$Y = 908.8 + 426.5X_1 + 1.8X_2 + 152.8X_3 + 37.8X_1X_2 + 133.0X_1X_3 + 137.0X_2X_3 + 65.6X_1^2 + 228.2X_2^2 + 171.7X_3^2$$



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Automated ANOVA & Pareto Analysis

Statistical Validation (ANOVA):

Metric	Value
R^2 / Adj. R^2	0.9716 / 0.9460
Model p-value	< 0.0001 (Significant)
Lack of Fit p	0.2579 (Not Sig. - Good)
Normality	$p = 0.8531$ (Shapiro-Wilk)
Dominant Factor	X_1 (57.19% Contribution)

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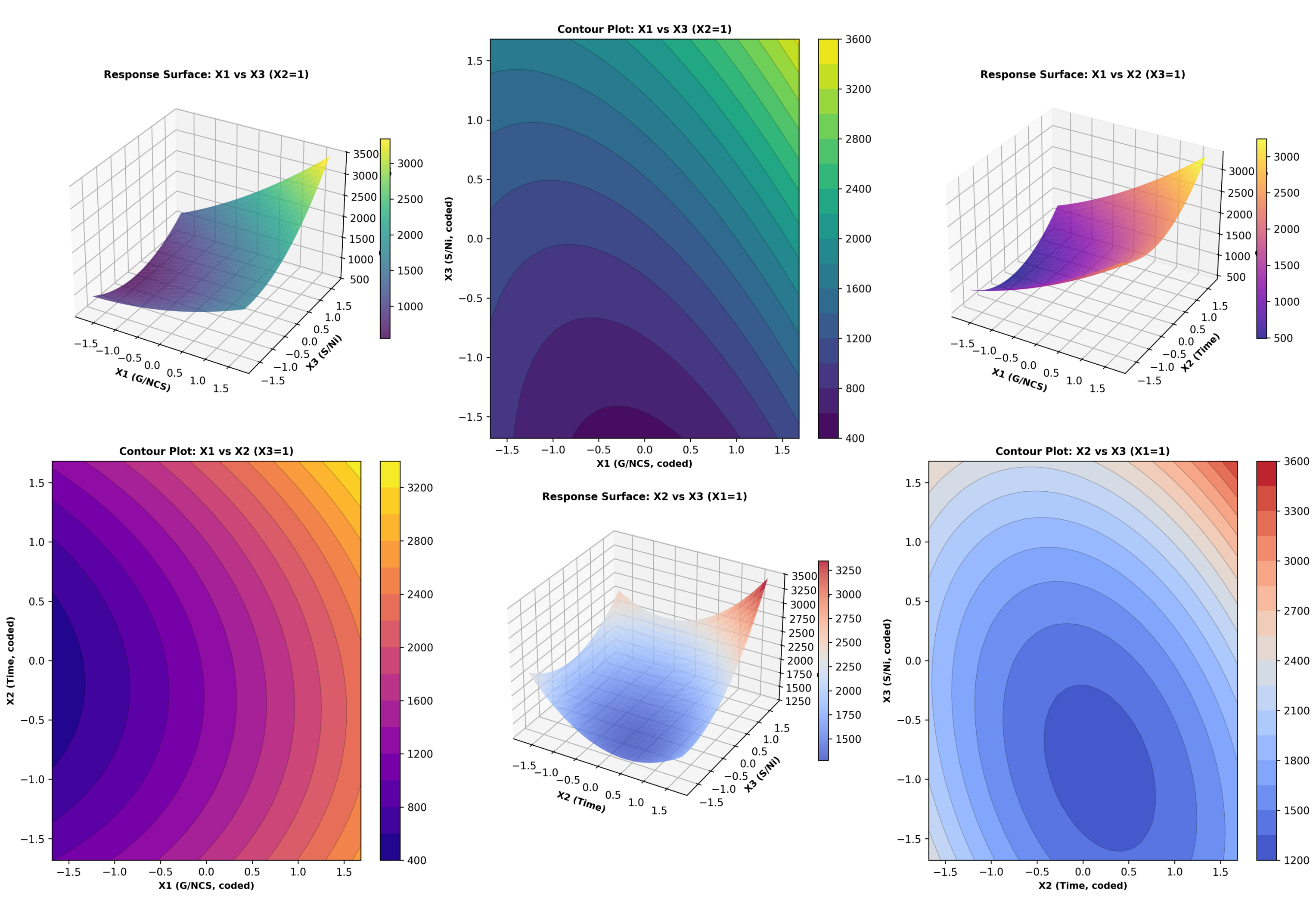
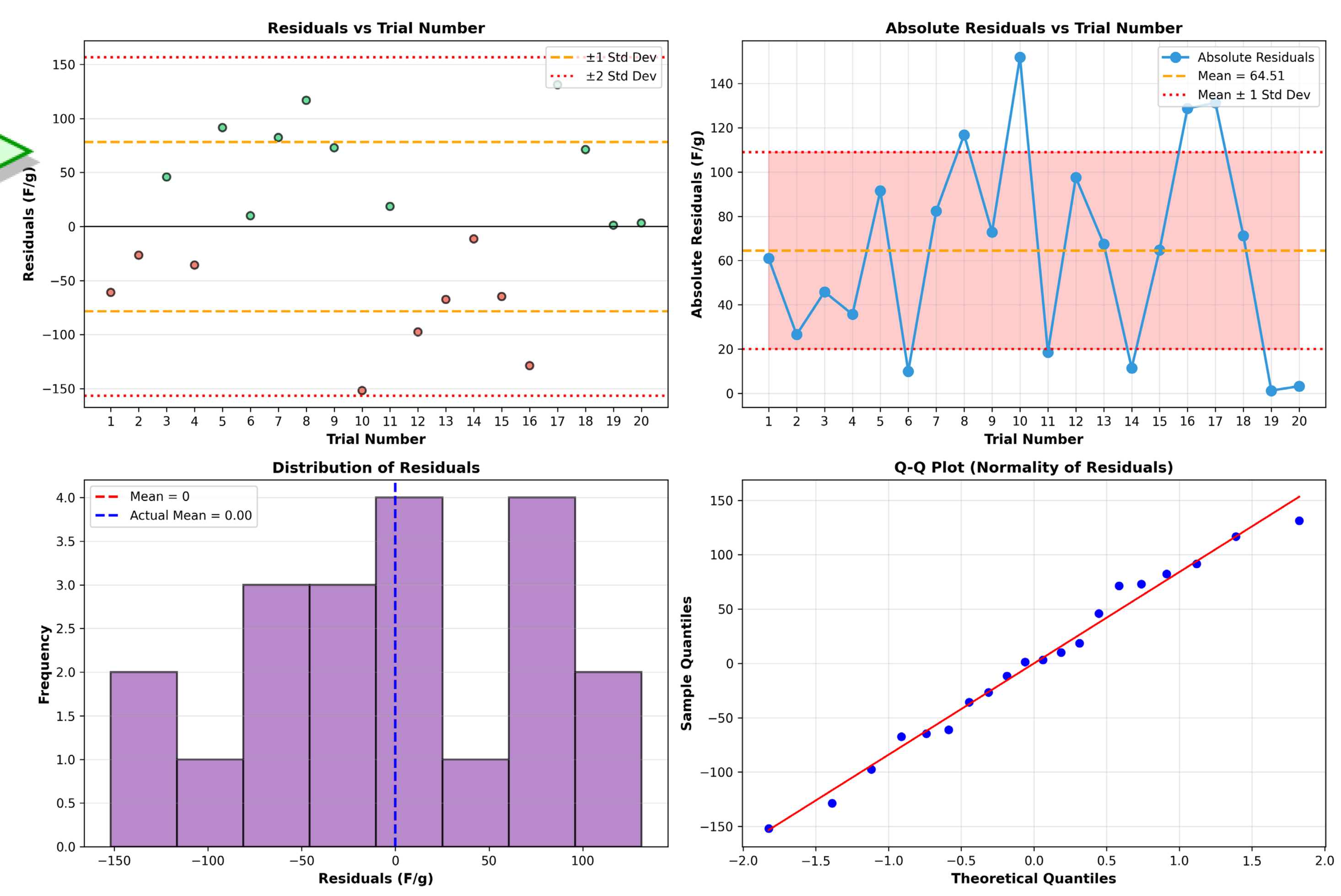
Model Valid? ($p < 0.05, R^2 > 0.9$)

No → Refine Model / Remove Terms





Yes ↓

Optimization Routine (Grid Search)

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Output: Optimal Conditions Maximization of Y

Global Optimal Solution:

- X_1 (G/NCS) = 6.0%
- X_2 (Time) = 10.0 h
- X_3 (S/Ni) = 6.0
- **Predicted Cap.: 2263 F/g**
- Deviation from Exp: 2.32%

CONCLUSION

The computational approach significantly reduces time investment while maintaining statistical validity, supporting industry adoption of data-driven design methodologies in energy storage materials. The complete Python code is provided as open-source supplementary material, enabling transparency, reproducibility, and broader methodological accessibility for future materials optimization research.

REFERENCES

[1] https://doi.org/10.3390/molecules27206867

[2] https://doi.org/10.1016/j.synthmet.2025.117844