Accelerating Nanocarbon Dispersion Research via Machine Learning and Automated Experimentation

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1. Introduction

The ability to process and organize nanomaterials in a controlled manner is essential for realizing their intrinsic properties and enabling reliable device integration. Solution processing through dispersion represents one of the most scalable approaches. However, identifying effective dispersants to create homogeneous and stable dispersions remains largely empirical because the quality of dispersion liquid depends on coupled effects of kind of dispersants and solvents, and processing conditions while the candidate chemical space is vast. Prior machine learning (ML) efforts in this area have often focused on narrower tasks (e.g., ranking solvents or optimizing process settings under fixed chemistries) rather than systematically discovering new dispersant molecules from broad libraries.[1] In this work, we present an ML-driven framework ("Dispersant Explorer") that treats dispersant discovery for carbon nanotubes (CNTs) as a data-driven search over open chemical databases using descriptors computed directly from Simplified Molecular Input Line Entry System (SMILES) alongside a small set of process descriptors.[2]

2. Experiments

We developed a data-driven framework, "Dispersant Explorer," to search open chemical databases for new dispersants targeting carbon nanotubes (CNTs). We derived descriptors from SMILES strings using RDKit, combining them with process features (e.g., sonication energy normalized for intensity). We trained a LightGBM regression model to predict dispersibility, as measured by optical density. An automated platform was configured to accelerate experimental validation. It cycles powder and liquid dosing, followed by horn-type ultrasonication, using a 4-axis robotic arm enabling reproducible data generation.

3. Results and Discussion

The model was applied to a broad chemical library, producing a ranked list of candidate dispersants under standardized conditions. Experimental validation confirmed that the model accurately predicted both high- and low-performing dispersants, including detecting subtle structural effects on CNT dispersion. We demonstrated the practical value of our discoveries by fabricating transparent conductive films (TCFs) from CNT dispersions using the top candidates. The films achieved best-in-class trade-offs between transmittance and sheet resistance for aqueous CNT-TCFs—attributable to the superior performance of the discovered dispersant.

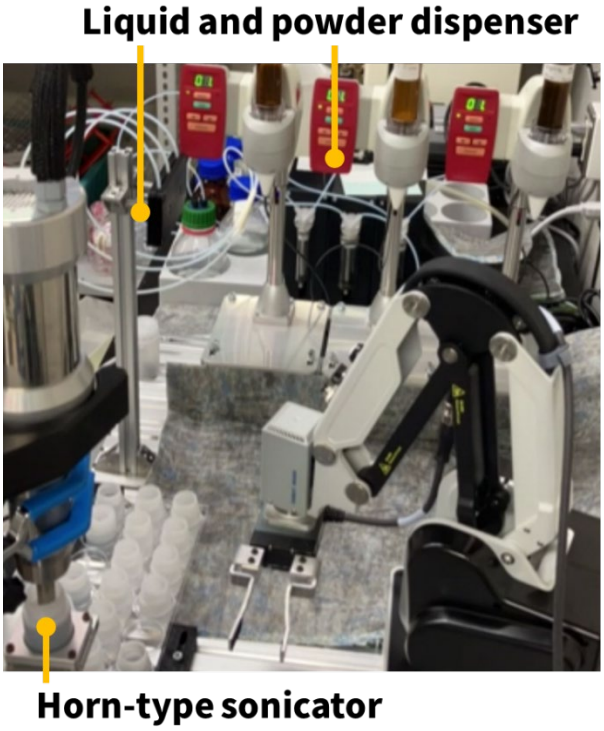

Fig. 1: Photograph of automated dispersion preparation system for nanomaterials, integrating powder/liquid dosing and ultrasonic treatment.

4. Conclusion

We present a LightGBM-based workflow for predicting aqueous carbon nanotube dispersants using a compact experimental dataset. By screening a wide range of organic molecules and experimentally validating selected candidates, we identified novel, high-performance

dispersants. Our integrated automation platform further accelerates and standardizes nanomaterial dispersion experiments.

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References

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