AI-Accelerated Discovery of High-Performance Thermoelectrics through Multi-Objective Optimization

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Optimizing thermoelectric (TE) materials means maximizing power factor ($PF = \alpha^2\sigma$) and figure of merit ($ZT = \alpha^2\sigma T/\kappa$). These require high Seebeck coefficient (α), high electrical conductivity (σ), and low thermal conductivity (κ), but these properties are interlinked, making simultaneous optimization very challenging. In this study, leveraging a 5-year experimental dataset of carbon nanotube yarn synthesis from a CREST project (JPMJCR18I3, Molecular Junction Approach for Wide-Range Control of Thermal Conductivity in Nano-Carbon-Based Materials), we treat each synthesis recipe as a "genome" (genes = synthesis variables) and apply a multi-objective evolutionary algorithm (NSGA-II) together with surrogate predictive models. The aim is to find Pareto-optimal recipes that balance PF and ZT, effectively navigating the trade-offs. We demonstrate how this AI-driven pipeline can rapidly suggest candidate recipes outperforming many human-designed ones, thereby accelerating the discovery cycle. While the case study is in thermoelectric yarns, the method generalizes to any domain with interdependent properties: drug discovery, electronics, thermal management, or materials for energy harvesting (e.g. converting waste heat to electricity). This work highlights how combining chemoinformatics, machine learning, and evolutionary search enables efficient discovery of high-performance materials, promising for both energy applications and translational materials chemistry.