ADVANCED DESIGN OF PIEZOELECTRIC MATERIALS FOR INTELLIGENT INFRASTRUCTURE APPLICATION

by

Guangshuai Han

A Dissertation

As infrastructure advances toward greater intelligence, piezoelectric materials play a vital role in converting mechanical performance into actionable data, facilitating better communication between humans and infrastructure to improve safety, operational efficiency, and sustainability. This work integrates computational and experimental approaches to advance the design of piezoelectric materials and devices for intelligent infrastructure applications. The research addresses three key areas: (1) optimizing piezoelectric performance at the molecular scale, (2) accelerating material discovery using artificial intelligence (AI), and (3) employing digital manufacturing techniques for enhanced piezoelectric sensors.

The first part of this work focuses on molecular-level strategies to enhance the piezoelectric performance of Polyvinylidene fluoride (PVDF), a polymer known for its flexibility but limited piezoelectricity. Using molecular dynamics simulations, the study explores how intermolecular forces, such as hydrogen bonding, align PVDF's dipole moments to optimize piezoelectric properties. This research establishes benchmark criteria for hydrogen bonding in PVDF systems—2.7 Å for hydroxyl groups and 3.2 Å for amino groups. Guided by these findings, the experimental synthesis of PVDF composites via co-axial electrospinning shows that Polypyrrole (PPy) as a dopant enhances the β-phase concentration to 97.6%, improving the piezoelectric d_{33} constant by 2.5 times.

Building on these molecular insights, the second phase of the work uses AI to accelerate piezoelectric material discovery. A highly accurate classification model was developed using an existing piezoelectric material database to predict piezoelectric performance. Applying this model to a broader crystal structure database identified 522 new potential piezoelectric materials, which were validated through theoretical calculations. This significantly enriches the piezoelectric material database and accelerates future discoveries.

The third section tackles the challenge of directional sensitivity in piezoelectric sensors. Traditional sensors detect forces from a single direction, but this research overcomes that

limitation by designing multi-channel sensors using additive manufacturing techniques. The foldable piezoelectric sensor developed enhances sensing across multiple directions, providing a robust solution for structural health monitoring in intelligent infrastructure.

Overall, this work presents advanced strategies for designing piezoelectric materials and devices by combining molecular-level optimization, AI-driven discovery, and innovative manufacturing techniques. These contributions provide a foundation for next-generation intelligent infrastructure, facilitating advanced monitoring solutions and driving progress in safety, sustainability, and operational efficiency.