Title: MXene-Based Self-Powered Flexible Sensors: Advances in Fabrication, Sensing Mechanisms, and Density Functional Theory-Driven Performance Optimization

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Abstract: As next-generation wearable electronics rapidly evolve, MXene-based self-powered textile sensors have emerged as a promising platform for integrating energy harvesting and multifunctional sensing within flexible textiles. MXenes offer exceptional electrical conductivity, tunable surface chemistry, strong hydrophilicity, and inherent mechanical flexibility, making them ideal for smart adaptive textiles. This review highlights recent progress in MXene synthesis and structural characterization and provides insights from density functional theory (DFT) into their electronic, optical, thermoelectric, and magnetic properties, thereby enhancing performance in energy harvesting and sensing. Fabrication and integration strategies, including coating, printing, electrospinning, and composite engineering, are discussed for scalable incorporation into textiles. Applications span motion and strain detection, tactile perception, gas and chemical monitoring, humidity and sweat sensing, and therapeutic or responsive fabrics. Despite advances, challenges persist, including oxidation, structural instability, limited washing durability, and the reliability of long-term measurements. Emerging solutions include hybrid nanostructures, protective encapsulation, AI-assisted optimization, and IoT-enabled architectures. These approaches aim to develop durable, washable, and sustainable MXene-based textiles for healthcare, sports monitoring, and human-machine interfaces, providing a roadmap for the practical deployment of self-powered wearable systems.

Keywords: density functional theory energy harvesting MXene piezoelectric nanogenerators self-powered sensors textile sensors triboelectricnanogenerators wearable electronics

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