# Defect-Driven Transport Phenomena in Energy and Functional Materials: A Comprehensive Review

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**Abstract:**
Defect-driven transport, involving ionic, electronic, and thermal carriers, is fundamental to the performance of many energy and functional materials. Intrinsic and extrinsic defects (vacancies, interstitials, substitutions) create pathways for ion migration and tune carrier concentrations, thereby controlling conductivity and reactivity. In complex oxides (e.g. perovskites) and solid electrolytes, oxygen or lithium vacancies greatly enhance ionic conduction. In thermoelectric materials (e.g. Bi–Te, Pb–Se alloys), controlled doping introduces charged defects that optimize carrier mobility and Seebeck coefficient. Two-dimensional materials (graphene, $MoS_2$, h-BN) can have their electronic band structure and conductivity tailored via atomic vacancies or substitutional dopants. We synthesise 2015–2025 theory and experiment to map structure–defect–transport relationships across classes, extract cross-cutting design principles (e.g., vacancy-mediated ion migration vs. dopant-controlled carrier density), and identify application-oriented strategies for fuel cells, solid-state batteries, thermoelectric modules, and 2D nanoelectronics. Unlike prior system-specific surveys, this review provides a unified framework that generalises mechanisms and trade-offs across material families while outlining verifiable performance baselines that defect engineering can achieve. We discuss key findings in perovskite oxides, halide perovskites, solid electrolytes, thermoelectrics, and 2D materials. Our synthesis reveals that oxygen vacancies in perovskite oxides and dopant-induced defects in thermoelectrics consistently enhance carrier mobility, while uncontrolled halide vacancies in solar cells degrade performance. Across all classes, moderate defect concentrations improve transport, but excess defect density introduces detrimental scattering. This review provides a unified overview of defect-driven ionic, electronic, and thermal transport across perovskite oxides, halide perovskites, thermoelectrics, solid electrolytes, and 2D materials. By correlating defect chemistry (type, concentration, and mobility) with transport phenomena, we highlight strategies that enable the

tailoring of conductivity and stability. Unlike previous reviews that focus on single material classes, this work emphasises cross-cutting mechanisms and proposes design principles to guide defect engineering in future energy devices.

**Keywords:**
Defect engineering, ionic conductivity, electronic transport, perovskite materials, solid electrolytes, thermoelectrics, energy materials, conductivity.