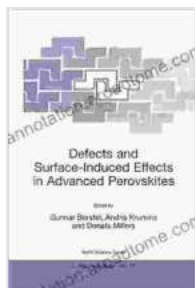


# Defects and Surface Induced Effects in Advanced Perovskites: A Comprehensive Exploration

Perovskites, a class of crystalline materials with the general formula  $ABX_3$ , have garnered immense attention in the scientific community due to their remarkable optoelectronic properties. Their exceptional light absorption, charge transport, and emission characteristics make them promising candidates for a wide range of applications, including solar cells, light-emitting diodes (LEDs), and photodetectors.



## Defects and Surface-Induced Effects in Advanced Perovskites: Proceedings of the NATO Advanced Research Workshop, Jurmala, Latvia, 23-25 August, 1999 (NATO Science Partnership Subseries: 3 Book 77)

by Daofeng He

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However, understanding and controlling the behavior of perovskites is crucial to optimize their performance and reliability. Defects and surface induced effects significantly influence the properties of these materials,

posing both challenges and exciting opportunities for researchers and engineers.

## Defects in Perovskites

Defects are imperfections in the crystal structure of perovskites that can arise during the growth process or under operating conditions. These defects can be classified into various types based on their dimensionality and origin:

- **Point Defects:** Isolated defects that occur at specific lattice sites, such as vacancies, interstitials, and substitutional impurities.
- **Line Defects:** One-dimensional defects, such as dislocations and grain boundaries, that disrupt the crystal structure over a localized region.
- **Planar Defects:** Two-dimensional defects, such as stacking faults and twin boundaries, that introduce additional interfaces within the crystal.

Defects in perovskites can impact their optoelectronic properties in several ways. For example, point defects can introduce energy states within the bandgap, affecting the absorption and emission of light. Line and planar defects can act as charge carrier traps, reducing the mobility and lifetime of charge carriers. Understanding and controlling defects is critical to enhance the performance and stability of perovskite-based devices.

## Surface Induced Effects in Perovskites

Perovskite surfaces are highly reactive due to the presence of dangling bonds and uncoordinated ions. This reactivity can lead to various surface induced effects that significantly impact the material's properties:

- **Surface Reconstruction:** The surface atoms rearrange to minimize the surface energy, resulting in a different crystal structure or composition compared to the bulk.
- **Surface Functionalization:** Molecules or ions can adsorb or react with the surface, modifying its electronic and chemical properties.
- **Surface Charge Accumulation:** Ions or electrons accumulate at the surface, creating an electric field and influencing the charge transport behavior.

Surface induced effects in perovskites are particularly important in applications where the surface plays a crucial role, such as in solar cells or photodetectors. By engineering the surface properties, it is possible to optimize charge extraction, improve device stability, and enhance the overall performance of perovskite-based devices.

## **Applications of Defects and Surface Induced Effects**

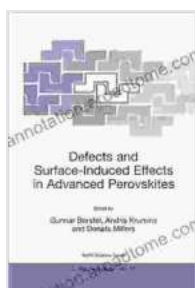
Understanding and controlling defects and surface induced effects in perovskites has opened up exciting opportunities for various applications:

- **Defect Engineering:** By intentionally introducing or modifying defects, researchers can tailor the optoelectronic properties of

perovskites for specific applications, such as tuning the bandgap or enhancing charge carrier transport.

- **Surface Passivation:** Modifying the surface of perovskites through functionalization or surface reconstruction can passivate defects and reduce surface recombination, improving device stability and performance.
- **Charge Transport Engineering:** Tailoring the surface properties of perovskites can control charge transport at interfaces, enabling efficient charge extraction and reducing energy losses in devices.

Defects and surface induced effects play a critical role in shaping the properties and applications of advanced perovskites. By understanding and controlling these phenomena, researchers and engineers can unlock the full potential of these promising materials for next-generation optoelectronic devices. Further research and advancements in this field hold immense promise for the development of high-performance, stable, and efficient perovskite-based technologies.



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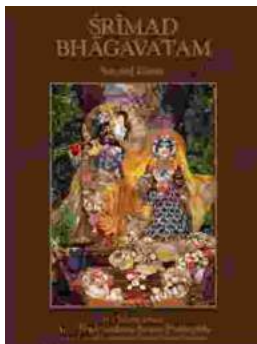
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