

# Chapter 6

## Perovskite Progress: the Role of Sr–Doping in Advancing BaTiO<sub>3</sub>– Based Technologies

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## ABSTRACT

*The incorporation of strontium into  $Ba_{1-x}Sr_xTiO_3$  compounds has a significant impact on their structural, electronic, optical, and mechanical properties. This study presents an analysis based on first principles calculations using density functional theory (DFT) to study the effects of strontium doping by varying Sr concentrations. The evolution of the structure, electronic band structures, optical and mechanical properties is examined to understand how Sr doping influences the fundamental characteristics of the material. The results highlight that Sr doping provides valuable information for tailored design of perovskite-type materials, thus optimizing their properties for various technological applications.*

## 1 BACKGROUND ON PEROVSKITE AND THE SIGNIFICANCE OF STRONTIUM DOPING IN $BaTiO_3$ -BASED TECHNOLOGIES.

### 1.1 Introduction on the perovskite material

Perovskite materials have become a primary area of interest in the field of materials science, thanks to their highly adaptable crystal structure and adjustable electronic properties. The standard formula for perovskite compounds is  $ABX_3$ , wherein 'A' and 'B' represent cations of distinct sizes, while 'X' denotes an anion that forms bonds with both (Roukos, 2015). This particular structure enables a multitude of chemical substitutions, rendering perovskites highly suitable for a broad spectrum of applications, ranging from solar cells to superconductors.

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