Chapter 6
Perovskite Progress: the Role of Sr-Doping in Advancing BaTiO3-Based Technologies

Hicham Kacimi-Naciri
Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS), Université Polytechnique Hauts-de-France, France & Laboratory of Process Engineering (LGP), Ibnou Zohr University, Agadir, Morocco

Mohamed Rguiti
Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS), Université Polytechnique Hauts-de-France, France

Assia Mabrouk
Higher School of Education and Training of Agadir, Ibnou Zohr University, Agadir, Morocco

Mohamed Aymen Ben Achour
Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS), Université Polytechnique Hauts-de-France, France

Yannick Lorgouilloux
Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS), Université Polytechnique Hauts-de-France, France

Christian Courtois
Laboratoire de Matériaux Céramiques et de Mathématiques (CERAMATHS), Université Polytechnique Hauts-de-France, France

Nadia Faska
https://orcid.org/0000-0001-6203-6904
Laboratory of Process Engineering (LGP), Ibnou Zohr University, Agadir, Morocco

Ahmed Bachar
Laboratory of Process Engineering (LGP), Ibnou Zohr University, Agadir, Morocco

DOI: 10.4018/979-8-3373-0669-8.ch006

ABSTRACT

The incorporation of strontium into Ba1-xSrxTiO3 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.

Fabrication and Evaluation of Superhydrophobic Surfaces Using Carbon Soot and Different Adhesives