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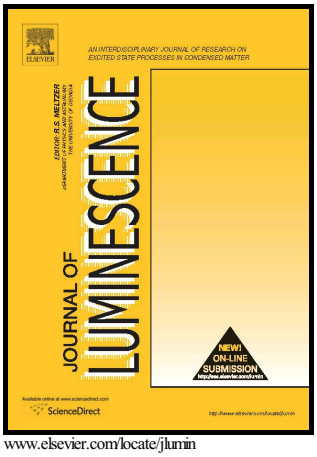

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A first-principles investigation on the luminescence emissions of $BaZrO_3$ obtained by microwave-assisted hydrothermal method

Rogério Almeida Gouvêa[a], Efrácio Mamani Flores[b], Sérgio da Silva Cava[a], Mário Lúcio Moreira[b,1]

[a] *CCAF, Programa de Pós-graduação em Ciência e Engenharia de Materiais, Centro de Desenvolvimento Tecnológico, Universidade Federal de Pelotas, Felix da Cunha, 809, CEP 96010-900, Pelotas, RS, Brasil*

[b] *CCAF, Instituto de Física e Matemática (IFM), Departamento de Física, Universidade Federal de Pelotas, Campus Capão do Leão, Caixa Postal, 354, CEP 96010-970, Pelotas, RS, Brasil*

Abstract

First-principles calculations were used as a tool to set the comprehension over radio-photoluminescence properties of $BaZrO_3$ prepared through microwave-assisted hydrothermal method. A systematic study of the influence of lattice defects on the electronic structure was carried out. Schottky, Frenkel and interstitial defects were taken into account in an attempt to find the midgap states responsible for luminescence. Barium and zirconium Schottky defects presented midgap states that can be associated to the photoluminescence emission while interstitial zirconium can lead to more stable medium range defects associated to the radioluminescence emission of barium zirconate. When both defects appear simultaneously the electronic structure is unable of luminescence emissions explaining the transition from photo to radioluminescence regime observed experimentally with synthesis time.

Keywords: $BaZrO_3$, microwave assisted hydrothermal, photoluminescence, radioluminescence, density functional theory

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*Corresponding author

Email address: mlucio3001@gmail.com (Mário Lúcio Moreira)