Influence of doped rare earth elements on electronic properties of the $R_{0.25}Ca_{0.75}MnO_3$ systems

Linh N.H., Trang N.T., Cuong N.T., Thao P.H., Cong B.T.

Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam; Faculty of Physics, Hue University of Education, Hue University, Viet Nam

Abstract: The influence of doped rare earth elements on the some electronic properties of perovskite systems $R_{0.25}Ca_{0.75}MnO_3$ (R = La, Nd, Eu, Tb, Ho, Y) is investigated using the density functional theory with Dmol3 code. The density of states, band structure, tolerance factor and Jahn-Teller splitting energy were calculated. By doping the different rare earth elements, the systems show different changing in the crystal structure, hopping amplitude, and electrical resistivity. Among these doping compounds, the $Eu_{0.25}Ca_{0.75}MnO_3$ exhibits the strongest structural change corresponding to the largest Jahn-Teller splitting. ?? 2010 Elsevier B.V. All rights reserved.

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Correspondence Address: Linh, N. H.; Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam; email: linknh@gmail.com

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Authors with affiliations:

1. Linh, N.H., Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam
2. Trang, N.T., Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam
3. Cuong, N.T., Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam

4. Thao, P.H., Faculty of Physics, Hue University of Education, Hue University, Viet Nam
5. Cong, B.T., Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Viet Nam

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