

Accepted Manuscript

Structural, elastic and optoelectronic properties of Sr-based perovskite-type oxides SrXO_3 (M=Th, Zr) via first-principles calculations

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PII: S0577-9073(18)30021-2
DOI: [10.1016/j.cjph.2018.06.002](https://doi.org/10.1016/j.cjph.2018.06.002)
Reference: CJPH 548



To appear in: *Chinese Journal of Physics*

Received date: 5 January 2018
Revised date: 2 April 2018
Accepted date: 2 June 2018

Please cite this article as: M.A. Ghebouli , T. Chihi , F. Dahmane , B. Ghebouli , M. Fatmi , T. Seddik , A. Abdiche , R. Khenata , Structural, elastic and optoelectronic properties of Sr-based perovskite-type oxides SrXO_3 (M=Th, Zr) via first-principles calculations, *Chinese Journal of Physics* (2018), doi: [10.1016/j.cjph.2018.06.002](https://doi.org/10.1016/j.cjph.2018.06.002)

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Highlights

- Some physical properties of SrXO_3 ($\text{M} = \text{Th}, \text{Zr}$) compounds have been investigated.
- The structural parameters and elastic constants agree well with the available data.
- Effect of pressure on the band gaps and some optical constants is predicted.

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