

055	UTBM service communication	Physics week	18 février 2014
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New Solids Research Findings from B. Bahloul and Colleagues Discussed

By a News Reporter-Staff News Editor at Physics Week -- Investigators publish new report on Solids Research. According to news reporting from Belfort, France, by VerticalNews journalists, research stated, "Structural, electronic and thermodynamic properties of SrTe and BaTe compounds and their ternary mixed crystals Ba(x)Sr1(-x)Te in the rock-salt structure have been studied with density functional theory (DFT), whereas the optical properties have been obtained by using empirical methods such as the modified Moss relation. The exchange-correlation potential was calculated using the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) and the local density approximation (LDA) of Teter-Pade (TP)."

The news correspondents obtained a quote from the research, "In the present work, we used the virtual-crystal approximation (VCA) to study the effect of composition (x). The calculated lattice parameters at equilibrium volume and the bulk modulus for x=0 and x=1 are in good agreement with the literature data. Furthermore, the BaxSr1-xTe alloys are found to be an indirect band gap semiconductor."

According to the news reporters, the research concluded: "In addition, we have also predicted the heat capacities (C-v), the entropy(S), the internal energy (U) and the Helmholtz free energy (F) of the parent compounds SrTe and BaTe."

For more information on this research see: Ab initio calculations of structural, electronic, optical and thermodynamic properties of alkaline earth tellurides BaxSr1-xTe. *Journal of Physics and Chemistry of Solids*, 2014;75(3):307-314. *Journal of Physics and Chemistry of Solids* can be contacted at: Pergamon-Elsevier Science Ltd, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, England. (Elsevier - www.elsevier.com; Journal of Physics and Chemistry of Solids - www.elsevier.com/wps/product/cws_home/229)

Our news journalists report that additional information may be obtained by contacting B. Bahloul, **UTBM** Univ, IRTES LERMPS FR FC Lab, Belfort, France. Additional authors for this research include A. Bentabet, L. Amirouche, Y. Bouhadda, S. Bounab, B. Deghfel and N. Fenineche.

Keywords for this news article include: France, Europe, Belfort, Solids Research

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Document number: news·20140218·QPABG·260

PUBLI-C news·20140218·QPABG·260

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Date d'émission : **2014-02-20**

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