MS16-P03 | STRUCTURE DESIGN OF NOVEL $Ba_{3-x}Sr_xTeO^6$ DOUBLE PEROVSKITES AND THE EFFECT OF TEMPERATURE AND COMPOSITION ON STRUCTURE STABILITY

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Double perovskite structure typically has the chemical formula $A_2BB'O_6$. Depending on the elements residing at A and B sites, different crystalline structures are possible. Fundamental understanding of the structure stability and phase transitions of these materials, under different synthesis conditions, is very important for optimizing the physical properties [1, 2].

In the present study, the mechanisms of self-doping together with continuous composition modulation in the $Ba_{3-x}Sr_xTeO_6$ ($0 \leq x \leq 3$) system are investigated. The structure stability and phase transition of compounds are studied using X-ray diffraction, and Raman spectroscopy at ambient and elevated temperatures. At ambient temperature, a systematic structure transition (*I*41/*a* → *R-3m* → *R-3*→ *R-3m* → *C*1) was determined, with x increasing from 0 to 3. At elevated temperatures (up to 570 °C) all structures tend to merge to the single cubic phase *Fm-3m*, indicating an expanded bonding length and a greater atomic thermal motion. The optical properties of the $Ba_{3-x}Sr_xTeO_6$ ($0 \leq x \leq 3$) system were part of the paper objective in investigating the substitution effect on the optical response. The optical properties of the compounds were significantly dependent to the symmetry change in the system and a shrink in the band gap energy values was observed as the amount of the strontium increase.

[1] Nielsen KK, Engelbrecht K, Andersen K. 2012;(May 2014). doi:10.1063/1.3695338
[2] Tamraoui Y, Manoun B, Mirinioui F, et al. J Mol Struct. 2017;1131.