

Abstract Submitted  
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**Stereochemical activity of lone-pair electrons in  $ABX_3$  heavy-element halides** YOUNG-MOO BYUN, EVA SMITH, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University —  $ABX_3$  halides display many functionalities and properties such as ferroelectricity and superconductivity.  $ABX_3$  (A = Rb, Cs; B = Sn, Pb; X = F, Cl) form generally in two different structures: sheelite ( $CaWO_4$ )-like and perovskite. The interplay of the stereochemically active lone pair (i.e., second-order Jahn-Teller) B-cation and other structural distortion is the key to determining the stable structure and subsequently the physical properties. It turns out that in these heavy p-block element compounds relativistic effects influence the activity of the lone pair in a nontrivial way. In this talk we will present our first-principles study of structural properties of this family of  $ABX_3$  halides and how they change with temperature and pressure.

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