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First-principles studies of lone-pair-induced distortions in epitaxial phases of perovskite $SnTiO_3$ and $PbTiO_3$[1] KRISHNA PITIKE, LYDIE LOUIS, University of Connecticut - Storrs, WILLIAM PARKER, Purdue University, SERGE NAKHMANSON, University of Connecticut - Storrs — In this project, a computational investigation utilizing density functional theory methods is carried out to elucidate the differences in stereochemical lone-pair activity of Pb and Sn A-site ions in epitaxial polar $ATiO_3$ perovskites. The contrasting tendencies for the lead- and tin-based compounds to form different phases under biaxial tension are connected to the amount of charge concentrated within the lone pair lobes. Specifically, phases are energetically more preferable when as much charge as possible is dissipated out of the lobe, thus lowering the cost of Coulomb repulsions between the lone pair and the surrounding oxygen cage. The insights gained about the electronic-level underpinnings of transitional behavior in such lone-pair active epitaxial ferroelectrics may be used in the design of a new generation of more efficient electromechanical and electrooptical devices.

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