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DFT investigation of structural effects on perovskites exhibiting metal-insulator phase transitions JOSEPH SCHICK, Villanova University, LAI JIANG, DIOMEDES SALDANA-GRECO, ANDREW RAPPE, University of Pennsylvania — The rich variety of electronic, magnetic, etc. properties available in perovskite materials are closely linked to octahedral tilting and other details of the arrangements of atoms within these materials. Furthermore, it has been demonstrated that the tilts and structural details are altered by the growth of films of these materials on substrates that provide strain and changed by the creation of new layered or superlattice structures from these materials. We employ density functional methods to investigate the relationship between tilting and charge ordering in a variety of strained-layered perovskite materials. We present these DFT results along with model calculations that aid in interpreting the complex connections between atomic structure and electronic properties, *e.g.* structural control of metal-insulator phase transitions.

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