# Density Functional Theory study on strain-dependent electronic structure at heterointerfaces of $CaSnO_3$ and $SrSnO_3$ with $SrTiO_3$

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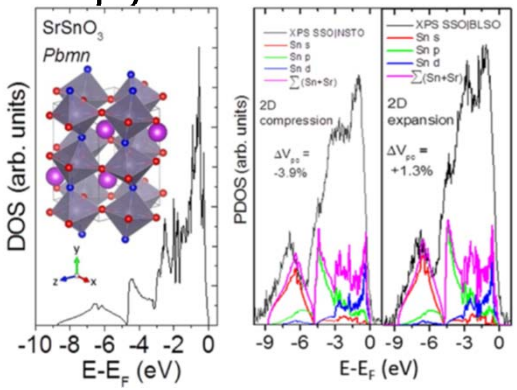
**Purpose** Elucidate the peculiarities of electronic structure and valence band alignment at heterointerfaces of strained epitaxial $ASnO_3$ thin films.

**Result** The valence band electronic structure is strain state dependent in a manner correlated with a directional change in Sn-O bond lengths with strain. The hybridized character of the Partial Density of States changes with volumetric strain in a manner consistent with the X-Ray Photoelectron Spectroscopy data.




## Computing system: VCC

| | |
|---|---|
| node-hour | about 400 node-hour of VCC |
| memory used | up to 50 GB |
| parallelize | up to 3 nodes of VCC |