

## **Symmetry, Stability and Electronic Etructure of Al, Sn and As Clusters**

**Raghani Pushpa and Umesh Waghmare**

We use density functional theory total energy and linear response calculations to study the structural instabilities in four and six atom high symmetry clusters of Al, Sn and As. We find that these instabilities arise from linear, quadratic and pseudo Jahn Teller couplings between the structural distortion and electronic states near HOMO. Based on analysis of these instabilities, we obtain a first principles model that captures anharmonicities in 4 atom Al clusters.