

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Stress induced tunable dielectric LiAsSe₂ FAN ZHENG, JOHN BREHM, STEVE YOUNG, ANDREW RAPPE, Univ of Pennsylvania — Tunable dielectric materials have many applications for the new electric devices. Traditionally, electric field is applied in order to tune the dielectric. We proposed a new material - LiAsSe₂ (space group *Cc*) as the potential tunable dielectric material. First-principle calculations show that with applying stress along [100] and [010] direction, dielectric constant can be enlarged by around factor of 3 depending on the stress magnitude. With calculated electronic structure, optical dielectric and absorption spectrum also show very large magnitude difference before and after applying stress. This large difference comes from the structure change. By shrinking in these two directions, the original alternating bonds length between neighboring As and Se atomic chain become even bonds. The top of valence band and bottom of conduction bands tend to exclusively contain Se p_z orbital and As p_z orbital. As a result, inter-band transition between these bands gives much larger transition dipoles. DFT+ U method is used in order to correct self-interaction error, especially to As atoms.

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Date submitted: 15 Nov 2013

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