Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A first principle approach using Maximally Localized Wannier Functions for computing and understanding elasto-optic reponse[1] XIN LIANG, SOHRAB ISMAIL-BEIGI, Yale University — Strain-induced changes of optical properties are of use in the design and functioning of devices that couple photons and phonons. The elasto-optic (or photo-elastic) effect describes a general materials property where strain induces a change in the dielectric tensor. Despite a number of experimental and computational works, it is fair to say that a basic physical understanding of the effect and its materials dependence is lacking: e.g., we know of no materials design rule for enhancing or suppressing elasto-optic response. Based on our previous work, we find that a real space representation, as opposed to a k-space description, is a promising way to understand this effect. We have finished the development of a method of computing the dielectric and elasto-optic tensors using Maximally Localized Wannier Functions (MLWFs). By analyzing responses to uniaxial strain, we find that both tensors respond in a localized manner to the perturbation: the dominant optical transitions are between local electronic states on nearby bonds. We describe the method, the resulting physical picture and computed results for semiconductors.

[1]This work is supported by the National Science Foundation through grant NSF DMR-1104974.

Xin Liang
Yale University

Date submitted: 11 Nov 2015 Electronic form version 1.4