Elasto-optic effect in semiconductors: a first principle approach using Maximally Localized Wannier Functions

XIN LIANG, SOHRAB ISMAIL-BEIGI, Applied Physics, 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 on this area, it is fair to say that a basic physical understanding of the effect and its materials dependence is lacking: for example, we know of no materials design rules for enhancing (or suppressing) elasto-optic response. Here, we begin by computing the elasto-optic tensor of silicon using Density Functional Theory (DFT). By analyzing the longitudinal dielectric response to uniaxial strain, we find that a promising avenue to physical understanding of the basis of the effect is to work in a real space representation and to employ Maximally Localized Wannier Functions (MLWFs). We describe our results based on this approach. This work is supported by the National Science Foundation through grant NSF DMR-0808665.