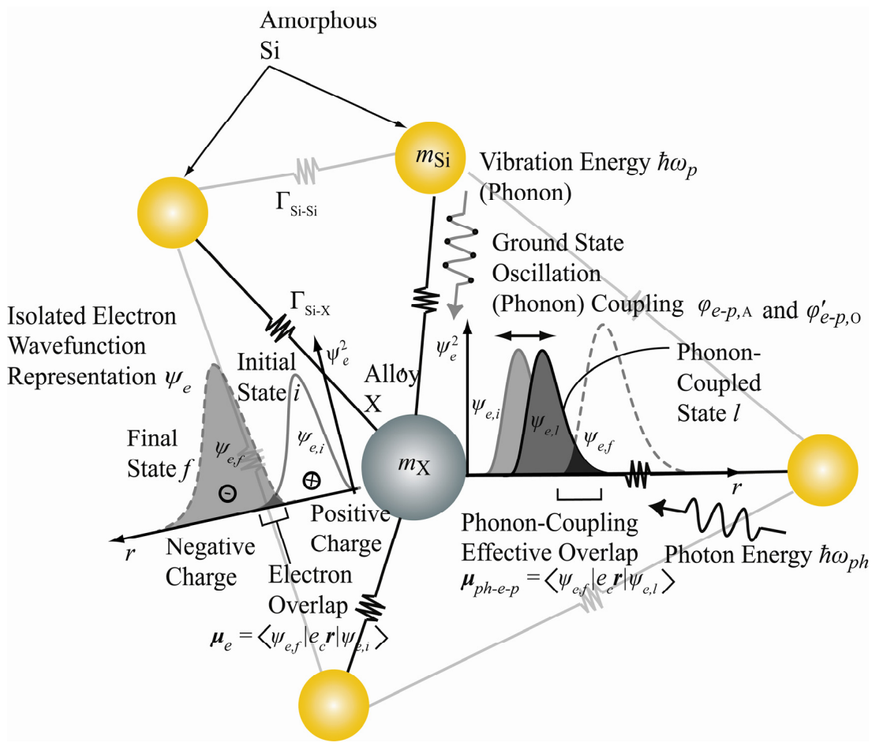
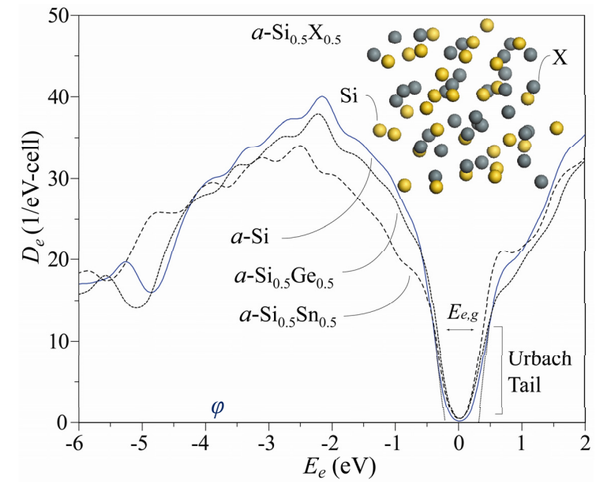
Photon-Electron-Phonon Interaction in Alloyed Amorphous Silicon

Using the observed temperature dependence of *a*-Si: H absorption spectrum and the second-order transition rate, phonon-coupled enhanced photon absorption is predicted for *a*-Si-X alloy. Phonons participated in the absorption process by oscillating the ground state electrons and create phonon coupled states. These states produce higher effective electron overlap between the ground and the excited state. We find that the electronic density of states is minimally altered by group IV elements while the phonon spectrum shows peak energy shift due to Si-X and X-X bond oscillations. *a*-$Si_{0.5}Sn_{0.5}$ alloy shows promising phonon-coupled photon absorption enhancement near the band-edge.



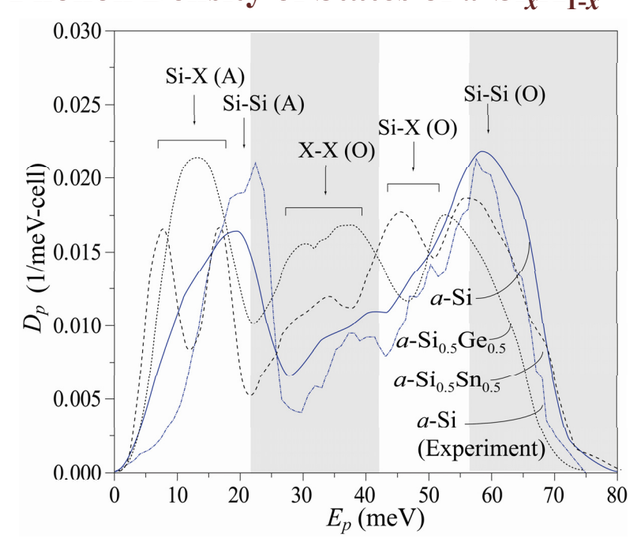
Conceptual rendering of photon-electron-phonon interaction in alloyed amorphous silicon. Due to broken symmetry, isolated electron representation can be used and the electronic wave-functions (ψ_e) are shown for initial (i), final (f), and phonon coupled state (l). Oscillations due to phonons create phonon coupled state (l) through acoustic and optical electron-phonon coupling constants $\varphi_{e-p,A}$ and $\varphi'_{e-p,O}$. These coupled states produce phonon-coupled effective electronic overlap $\boldsymbol{\mu}_{ph-e-p}$ which enhances the photon absorption.

Electronic Structure of *a*-Si_xX_{1-x}



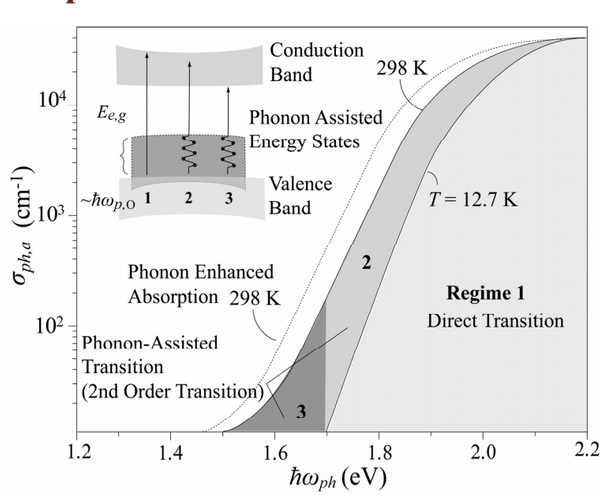
The electronic structure of *a*-Si_xX_{1-x}. The comparison of the density of states D_e show that even with high X content (group IV elements), the overall density distribution near the band-edge is virtually unchanged. This is because most of the electronic density is known to be composed of *s* and *p* orbitals near the band-gap which is retained in the a-Si_xX_{1-x}. This shows that D_e is not sensitive to the type of the element but on the coordination of the atoms. However, for Sn, the results indicate a smaller band-gap which may be advantageous in increasing the energy conversion efficiency.

Phonon Density of States of *a*-Si_xX_{1-x}



The phonon density of states of *a*-Si_xX_{1-x}. When element X is added, the lower phonon energy peaks (due to Si-X and X-X) appear. As the phonon peak energy decreases, the occupation probability of these modes increase (due to boson function) which predict enhancement of the phonon-coupled photon absorption and the overall absorption coefficient. Unlike D_e, D_p shows significant dependence on the alloying element, indicating that the phonon spectrum is readily altered by composition.

Absorption Coefficient of *a*-Si: H



The absorption spectrum of a-Si: H . Near the band-edge, *a*-Si H shows significant temperature dependence and a direct band-gap like behavior. However, the actual band-to-band transition is indirect but phonons freely couple during the photon absorption process due to broken symmetry (no momentum selection rule exists). Single photon absorption (direct) is dominate at low temperatures but phonon-assisted photon absorption is also significant at high temperatures. When phonon participation is enhanced, the absorption coefficient will increase without any increase in temperature.