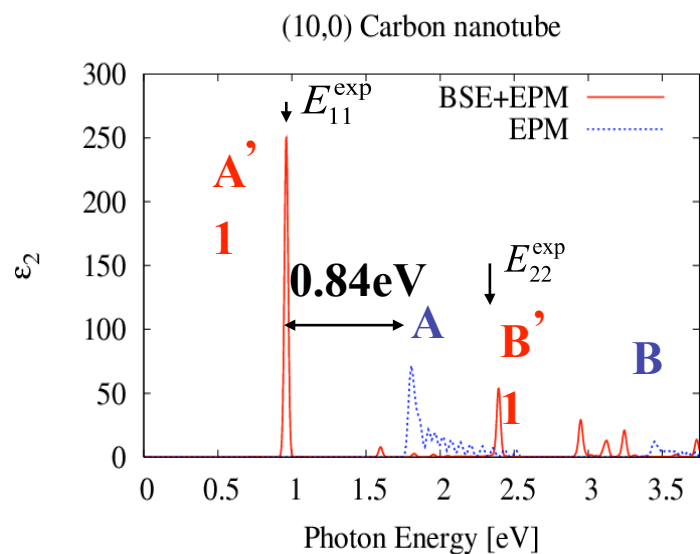
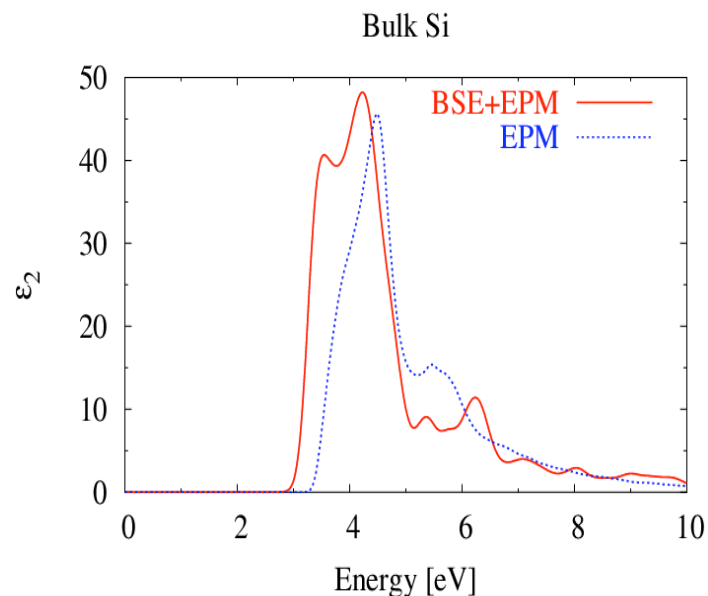


Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steve Louie (UC Berkeley) and Efthimos Kaxiras (Harvard)
(DMR- 0551195): Optical Absorption and Excitonic Effects in Nanostructures



Owing to their low-dimensionality, excitonic effects are very important in describing the optical properties of nanomaterials.

To investigate the optical spectra and excitonic effects of nanostructured materials, we solve the Bethe-Salpeter equation of the two-particle Green's function employing one-particle input from the empirical pseudopotential method (EPM), which is computationally much more efficient than using one-particle input from the GW approximation, although the EPM is less accurate. As shown in the figures, the excitonic effect is indeed important in nanotubes, as well as in bulk Si.

The calculated absorption spectra agree quite well with experiments and ab initio results. The current method can be efficiently used for investigating the optical properties of nanomaterials, which contain large numbers of atoms, so that ab initio methods cannot be used.