Optical investigations using ultra-soft pseudopotential calculations of Si0.5Ge0.5 alloy

Ultra-soft pseudopotential (US-PP) calculations with a powerful package called VASP (Vienna ab initio simulation package) are used. The total density of state and the energy gap of $Si_{0.5}Ge_{0.5}$ alloy of zinc-blende structure are calculated using the band structure scheme. The energy gap is found to be indirect for the zinc-blende structure. The results of refractive index and optical dielectric constant of $Si_{0.5}Ge_{0.5}$ alloy are investigated. The results are in reasonable agreement with experimental and theoretical ones.