# First principle study of the plasmon modes of diamond under pressure through energy loss spectrum

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## Abstract

In this paper by using first principle method we address the variation of bulk plasmon frequencies of diamond crystal underlying hydrostatic pressure in the rang 0-100 GPa. Further, optical properties such as reflectivity coefficient is also calculated. Based on electronic structure, density of transition probability and electron energy loss function results show that by increasing the pressure to 100 GPa, plasmon excitation shifts to higher energies about 4 eV in the near ultra-violet regime along with increasing the electronic band gap. That is while enhancing the pressure would reduce the plasmon lifetimes via the formation of electron-hole pair. Our finding shows that the modulation of all optical features such as collective plasmonic excitations are possible by manipulation and control of dielectric function by external probes such as mechanical pressure.

**Keywords:** Time Dependent Density Function Theory (TDDFT), Plasmon excitation, Full Width at Half Maximum (FWHM), Electron Energy Loss Function (EELS), Reflection constant, Diamond

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