Supporting Information

Microscopic origin of pressure-induced phase-transitions in urea: A detailed investigation through first principles calculations

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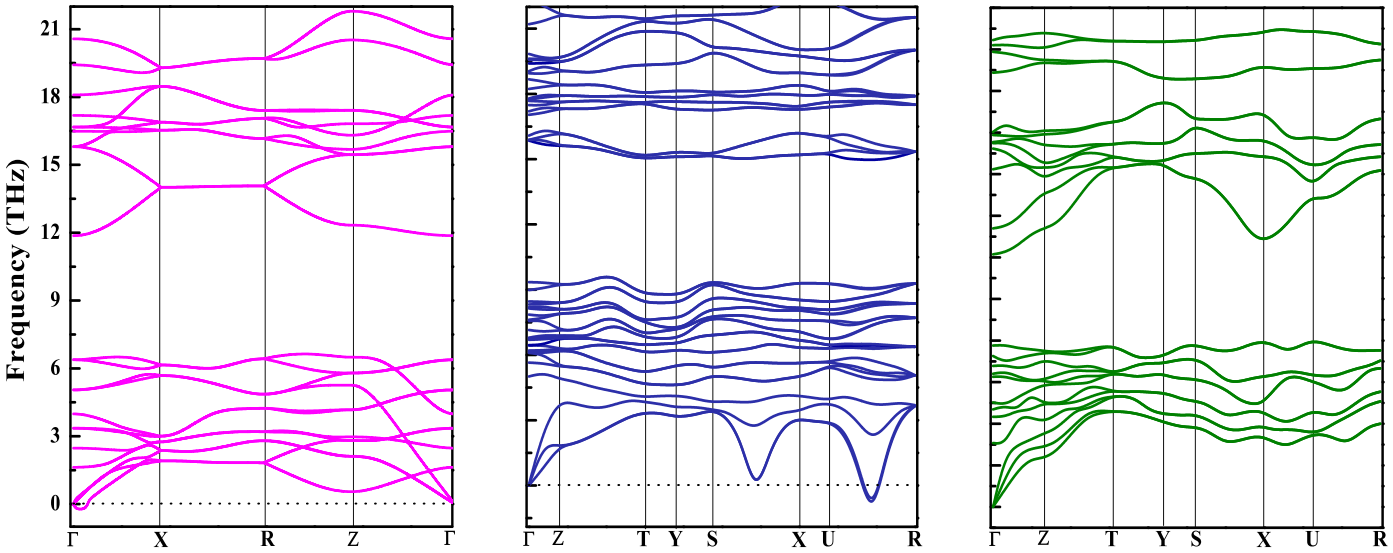

(a) (b) (c)

Figure 1: (Color online) Calculated phonon dispersion spectrum for (a) phase I (at 0.66 GPa), (b) phase III (at 3.09 GPa) and (c) phase IV (at 4 GPa) of urea polymorphs.

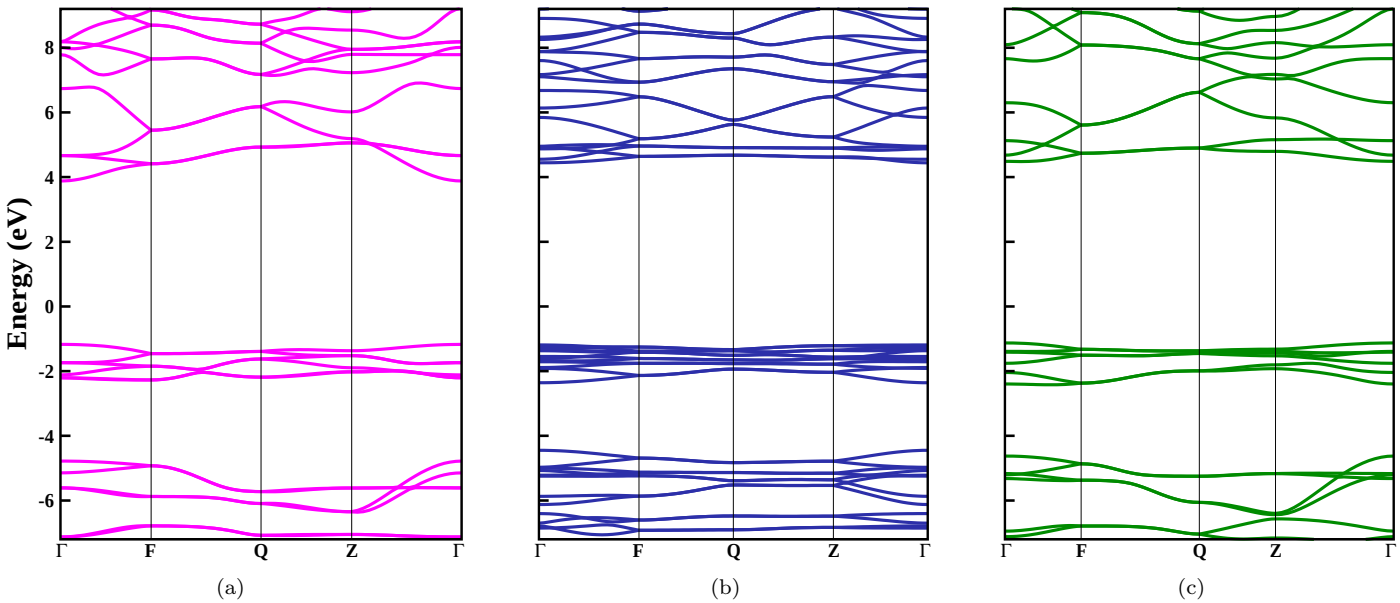

Figure 2: (Color online) Calculated band structures using PBE-GGA functional for (a) phase I, (b) phase III and (c) phase IV at 0, 0.66 and 3.09 GPa, respectively.

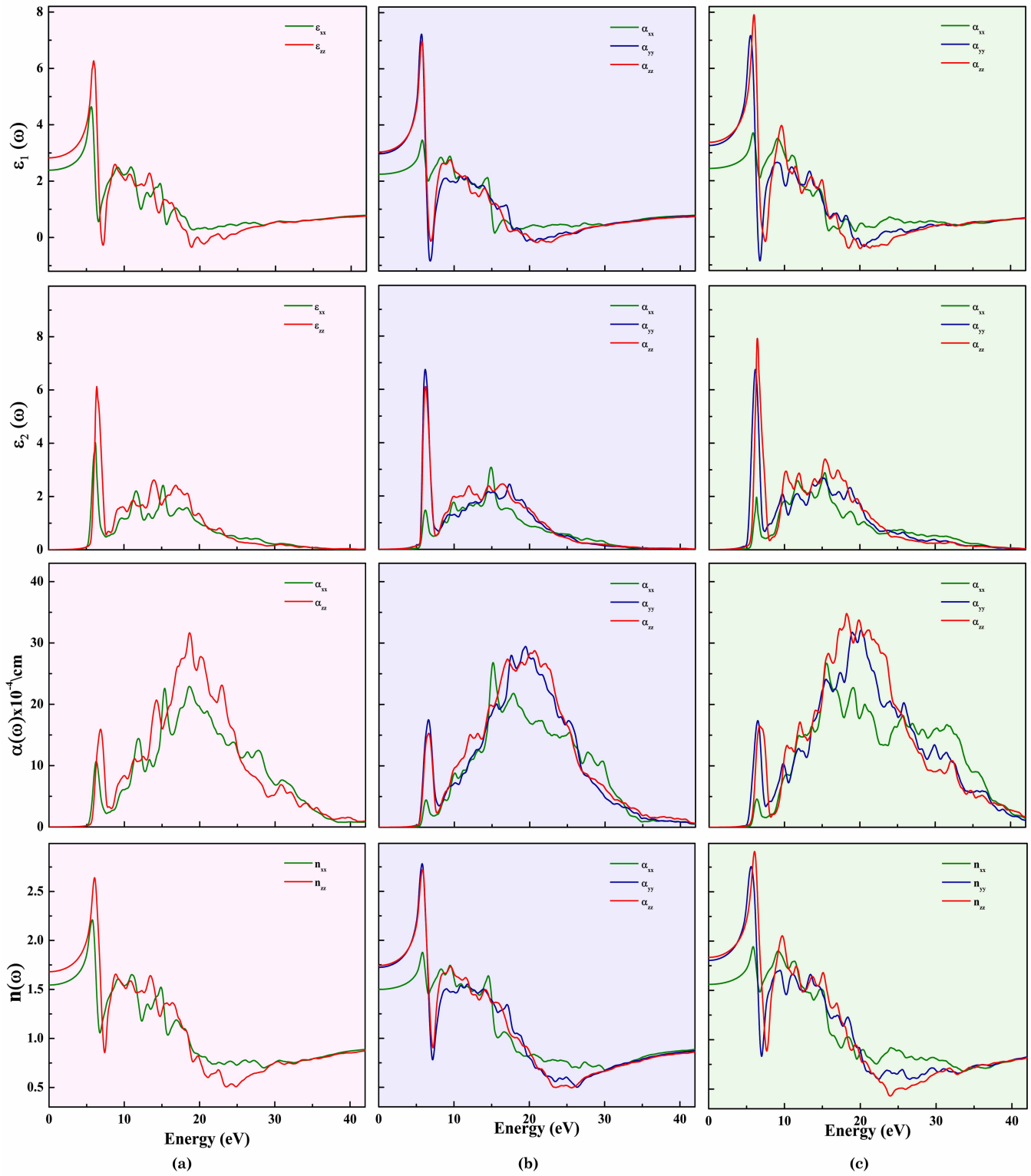

Figure 3: (Color online) Optical spectra (dielectric functions (real ($\epsilon_1(\omega)$) and imaginary ($\epsilon_2(\omega)$) parts), absorption spectra and refractive index of urea polymorphs as a function of photon energy calculated using PBE-GGA method for (a) phase I, (b) phase III and (c) phase IV at 0, 0.66 and 3.09 GPa, respectively.