Supplementary Information to

First-principles study of structural, elastic, electronic and optical properties of RDX under pressure

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**Fig. S1.** Calculated elastic constants of α-RDX as functions of pressure.



**Fig. S2.** Calculated bulk modulus, shear modulus and Young’s modulus as functions of pressure.



**Fig. S3.** The complex dielectric function of α-RDX for polarization direction (100), (010) and (001) under pressure from 0 to 40 GPa.



**Fig. S4.** The complex refractive index of α-RDX for polarization direction (100), (010) and (001) under pressure from 0 to 40 GPa.



**Fig. S5.** Theoptical reflectivity of α-RDX for polarization direction (100), (010) and (001) under pressure from 0 to 40 GPa.



**Fig. S6.** The energy-loss spectrum of α-RDX for polarization direction (100), (010) and (001) under pressure from 0 to 40 GPa.



**Fig. S7.** The complex conductivity of α-RDX for polarization direction (100), (010) and (001) under pressure from 0 to 40 GPa.

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