Supplementary information for "Dual-Surface Functionalization of Graphene beyond DFT Limits: Nanoscale Insights into Flat Bands and Optical Behavior"

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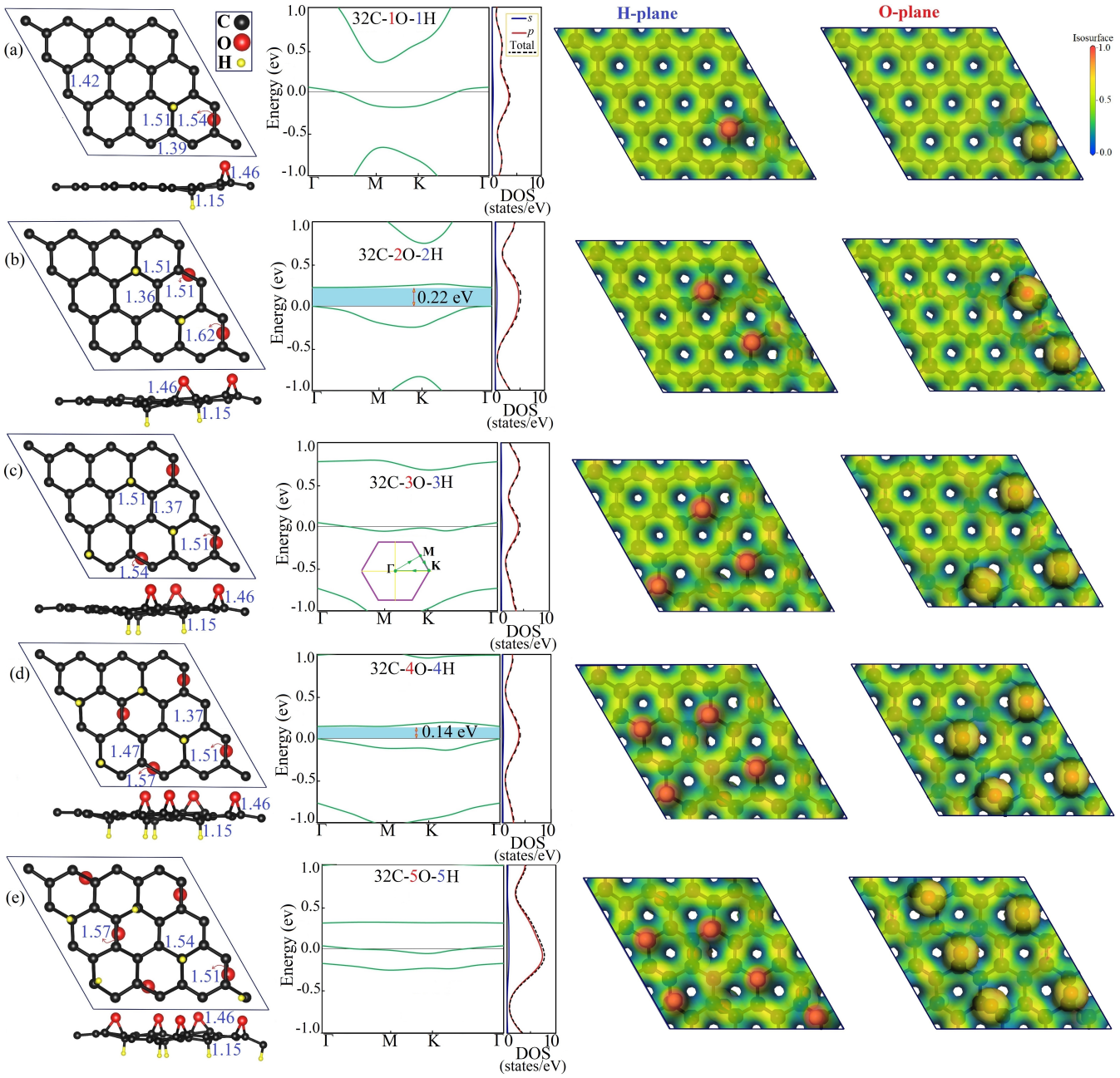

FIG. S1. The computed properties of zC-xH-yO (z=32, x, y= 1-5): (Left) Top and side views of the optimized supercell. The bond lengths are in Å. (Middle) The electronic band structure and the electronic density of states (DOS). The panel shows the First Brillouin zone (FBZ). (Right) Electron localization function (ELF) from top views of planes containing H and O atoms.

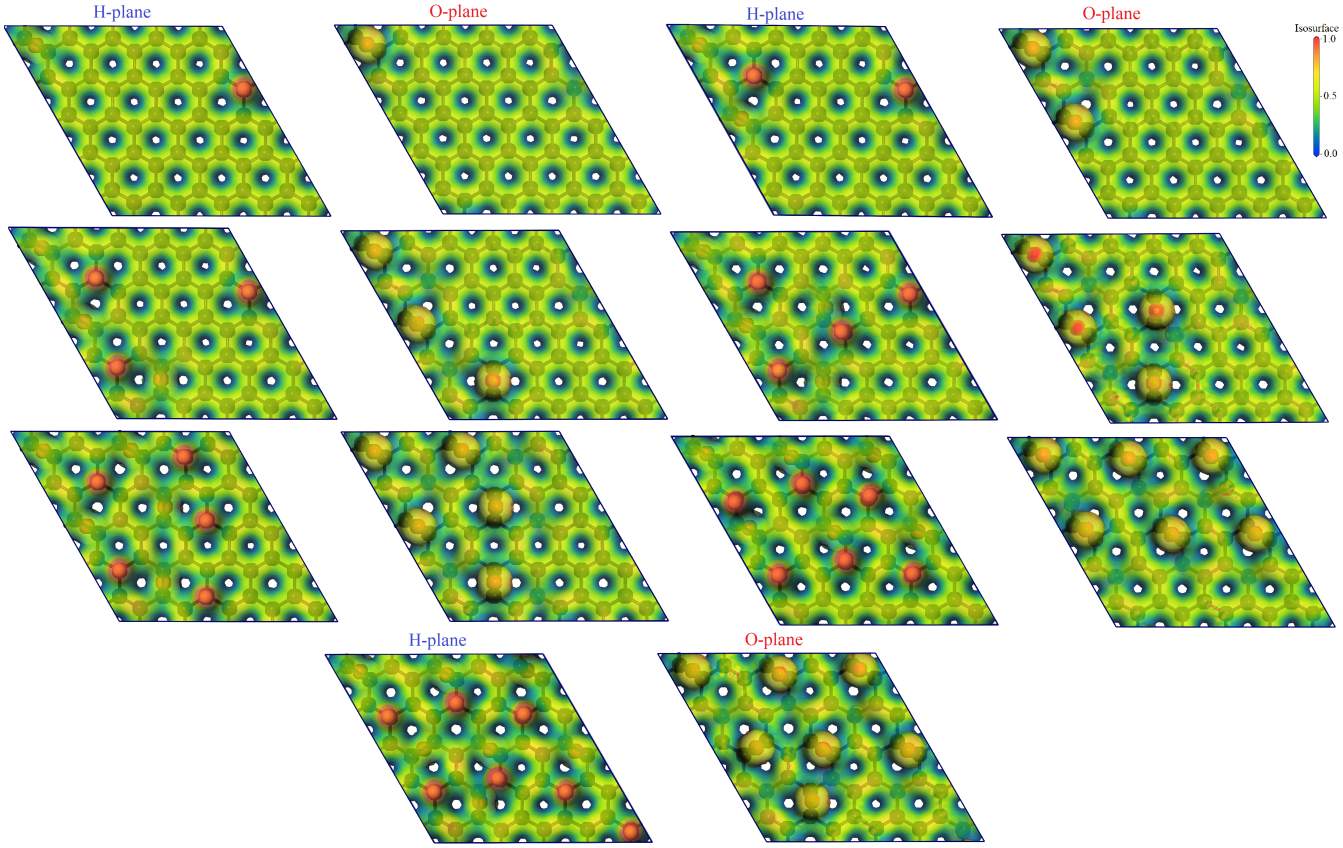

FIG. S2. Electron localization function (ELF) from top views of planes containing H and O atoms of the zC-xH-yO (z=50, x, y= 1-7) structures.

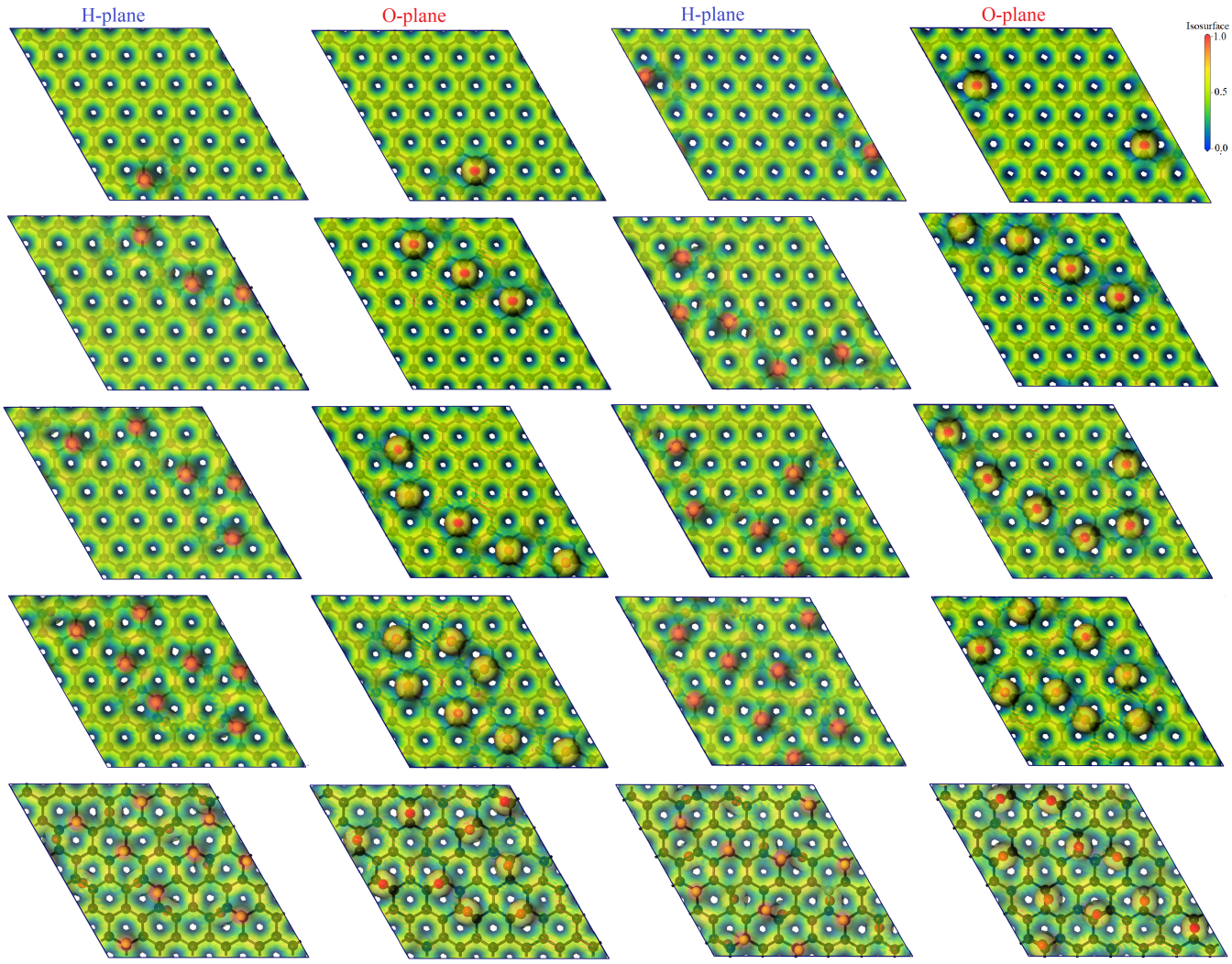

FIG. S3. Electron localization function (ELF) from top views of planes containing H and O atoms of the zC-xH-yO (z=72, x, y= 1-10) structures.

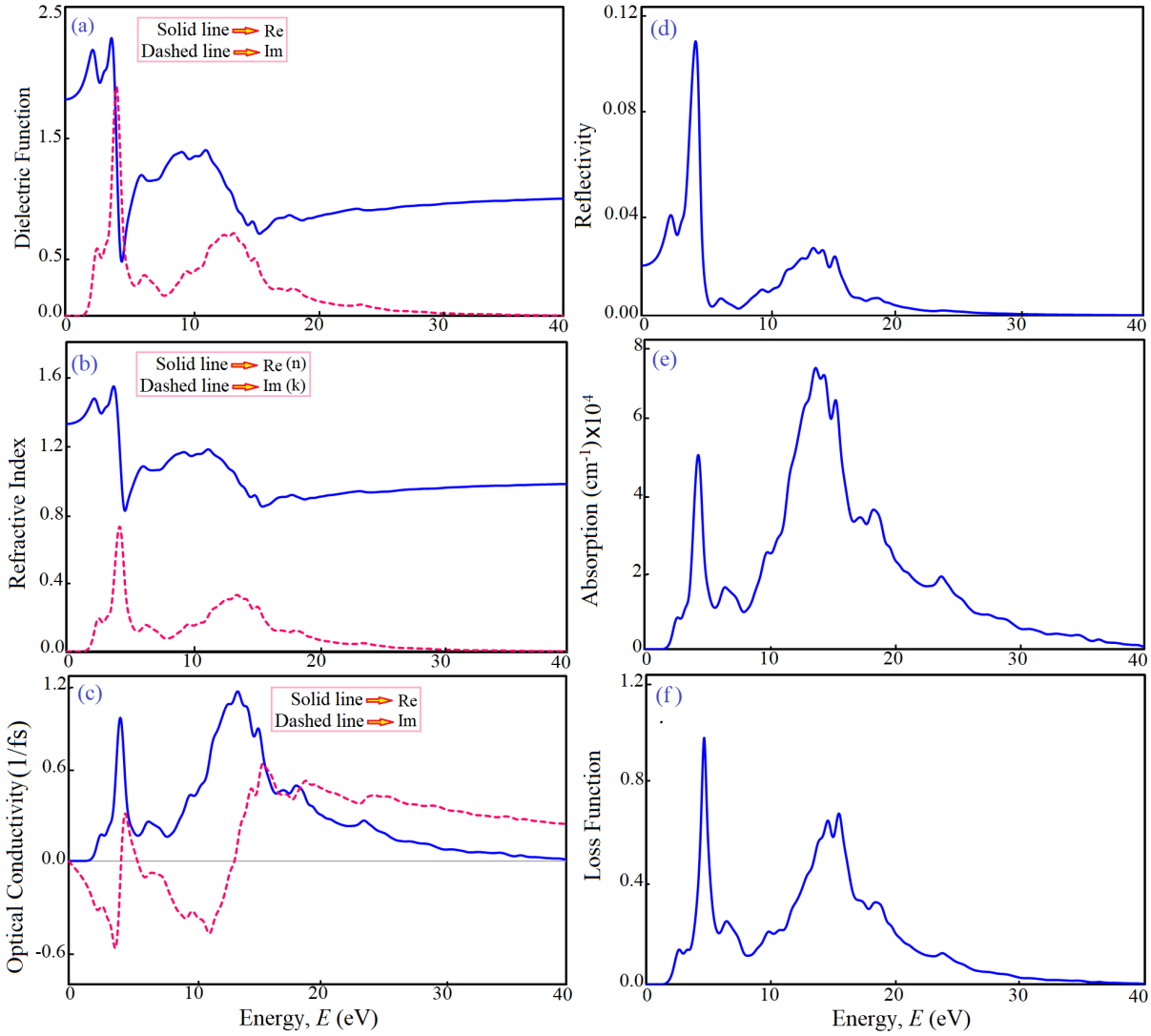

FIG. S4. (a) Dielectric function, (b) refractive index, (c) optical conductivity, (d) reflectivity, (e) Absorption, and (f) loss function of the zC-xH-yO (z=8) structures.

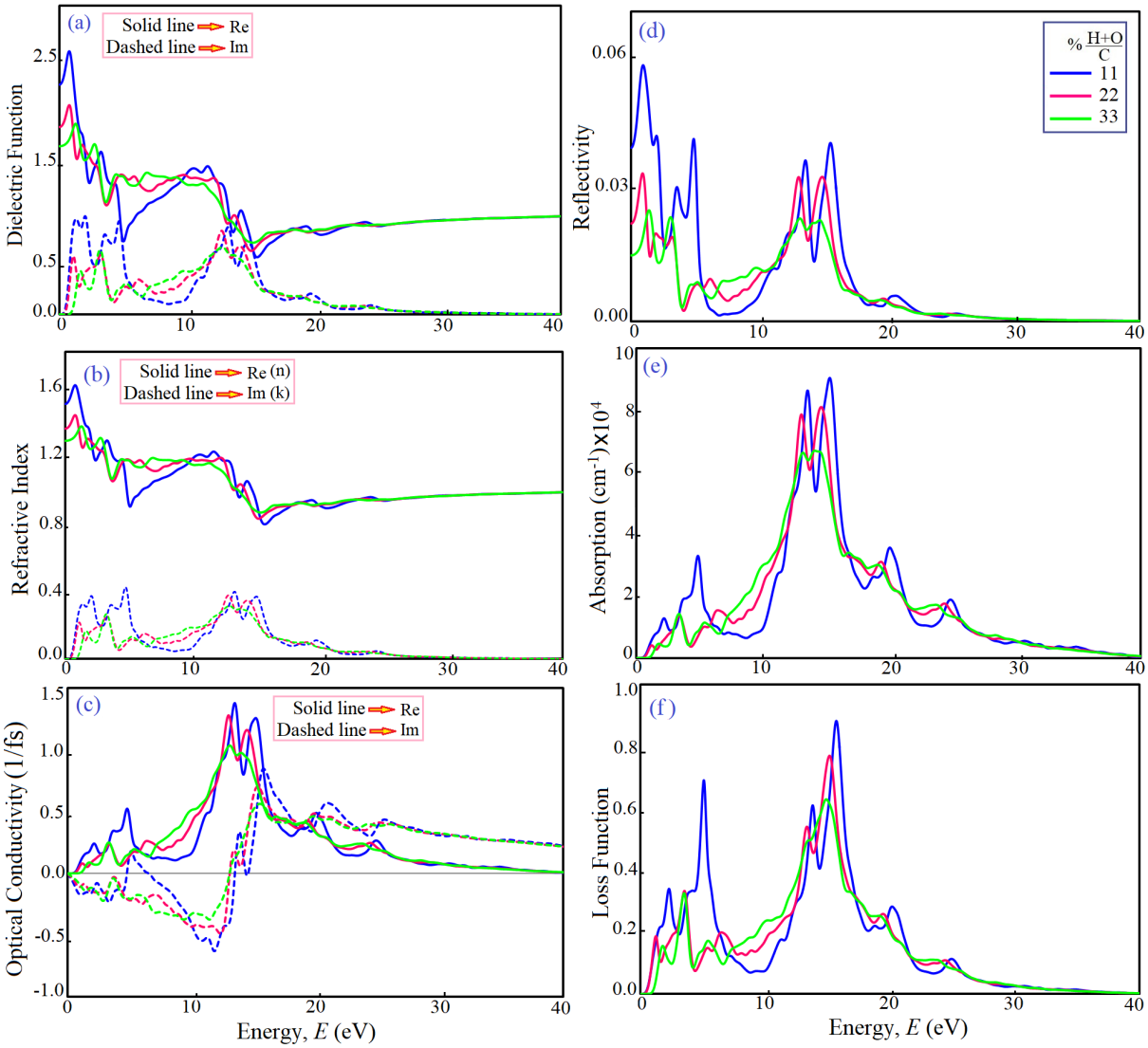

FIG. S5. (a) Dielectric function, (b) refractive index, (c) optical conductivity, (d) reflectivity, (e) Absorption, and (f) loss function of the zC-xH-yO (z=18) structures.

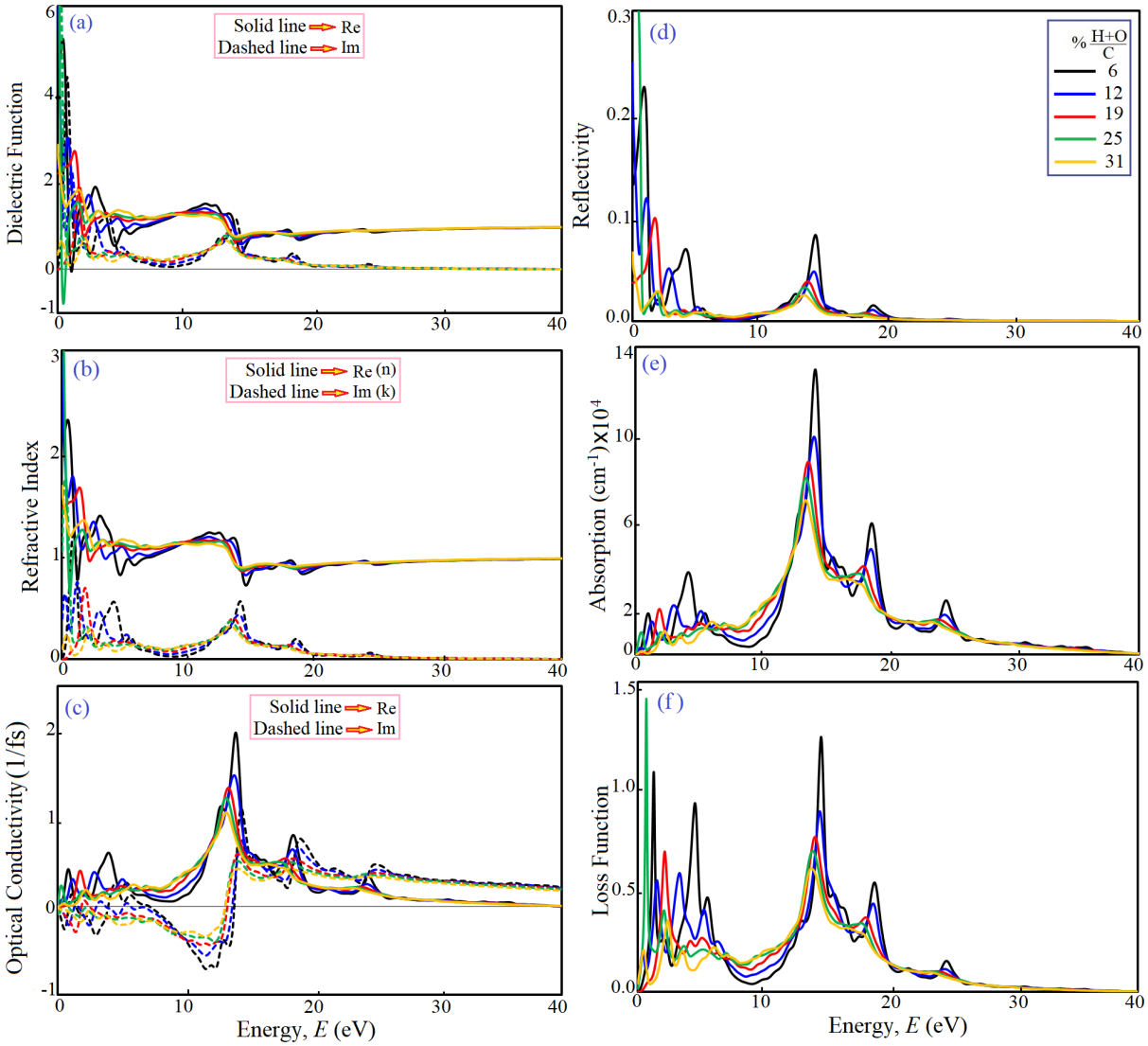

FIG. S6. (a) Dielectric function, (b) refractive index, (c) optical conductivity, (d) reflectivity, (e) Absorption, and (f) loss function of the zC-xH-yO (z=32) structures.

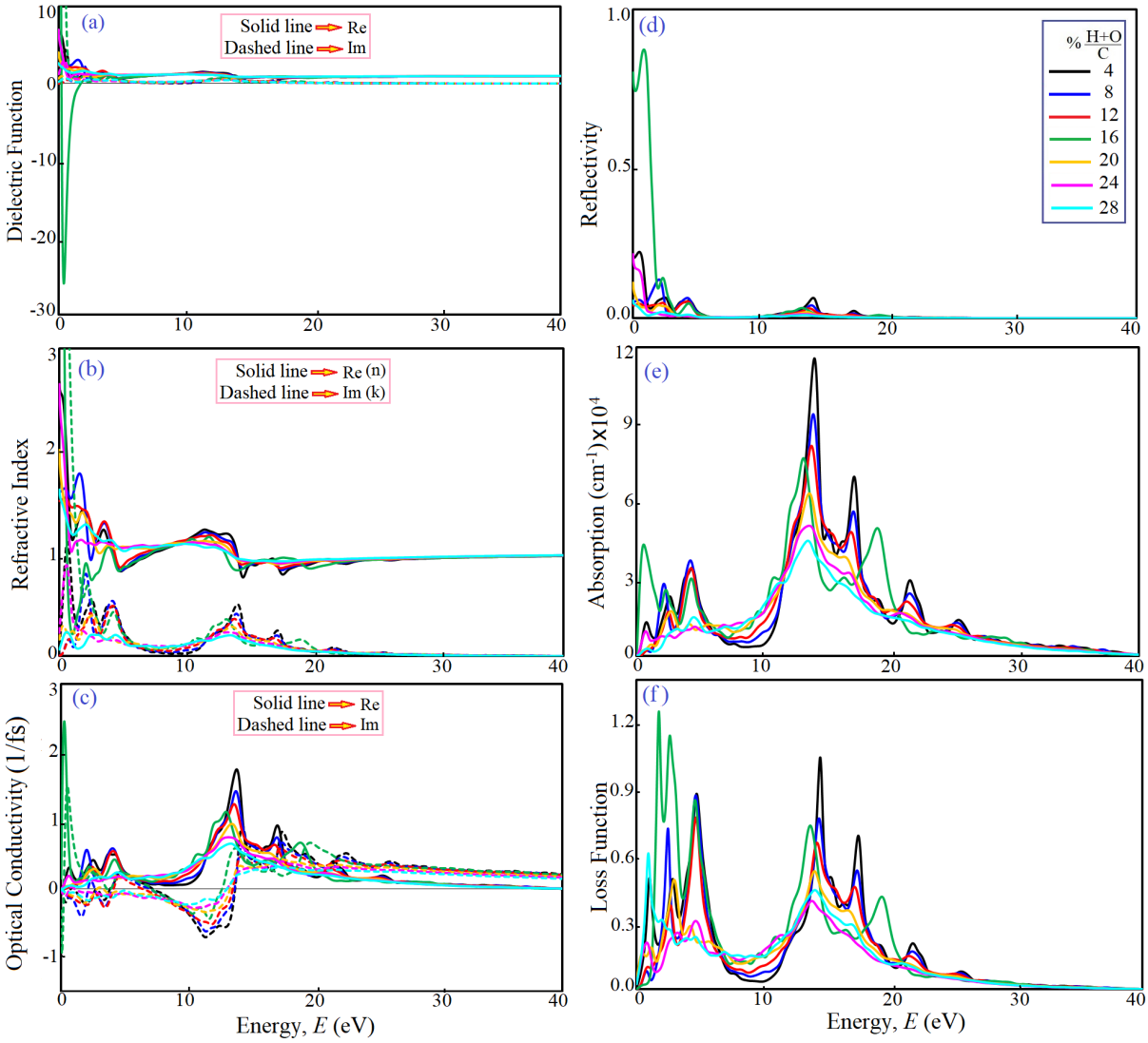

FIG. S7. (a) Dielectric function, (b) refractive index, (c) optical conductivity, (d) reflectivity, (e) Absorption, and (f) loss function of the zC-xH-yO (z=50) structures.