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Revisiting isoreticular MOFs of alkaline earth metals: A comprehensive study on phase stability, electronic structure, chemical bonding, and optical properties of A-IRMOF-1 (A = Be, Mg, Ca, Sr, Ba)

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Supplementary Material (ESI) for PCCP

Table S1. Optimized bond length (Å) and bond angles (°) for A-IRMOF-1 (A = Be, Mg, Ca, Sr, or Ba) at their equilibrium volumes[a]

A	C1-C2 (Å)	C2-C3 (Å)	C3-C3 (Å)	C1-O2 (Å)	A-O1 (Å)	A-O2 (Å)	O2-A-O2 (°)
Be	*1.490*, **1.491**	*1.404*, **1.404**	*1.391*, **1.391**	*1.274*, **1.274**	*1.717*, **1.717**	*1.634*, **1.635**	*102.905*, **102.921**
	<1.468>	<1.388>	<1.377>	<1.262>		<1.602>	<102.812>
Mg	*1.496*, **1.496**	*1.404*, **1.404**	*1.391*, **1.391**	*1.277*, **1.276**	*1.989*, **1.989**	*1.959*, **1.960**	*108.332*, **108.339**
	<1.472>	<1.388>	<1.377>	<1.265>		<1.903>	<108.210>
Ca	*1.499*, **1.500**	*1.404*, **1.403**	*1.391*, **1.391**	*1.277*, **1.277**	*2.270*, **2.270**	*2.242*, **2.242**	*112.455*, **112.459**
	<1.476>	<1.389>	<1.377>	<1.266>		<2.125>	<111.751>
Sr	*1.502*, **1.502**	*1.403*, **1.403**	*1.392*, **1.392**	*1.276*, **1.276**	*2.433*, **2.434**	*2.406*, **2.406**	*114.125*, **114.125**
Ba	*1.504*, **1.504**	*1.403*, **1.403**	*1.392*, **1.392**	*1.276*, **1.276**	*2.607*, **2.607**	*2.579*, **2.580**	*115.537*, **115.529**

[a] The bond lengths and angles in italic and bold fonts are from **Γ**-point and 2×2×2 **k**-point calculations, respectively. Data in <braces> are from ref 9.

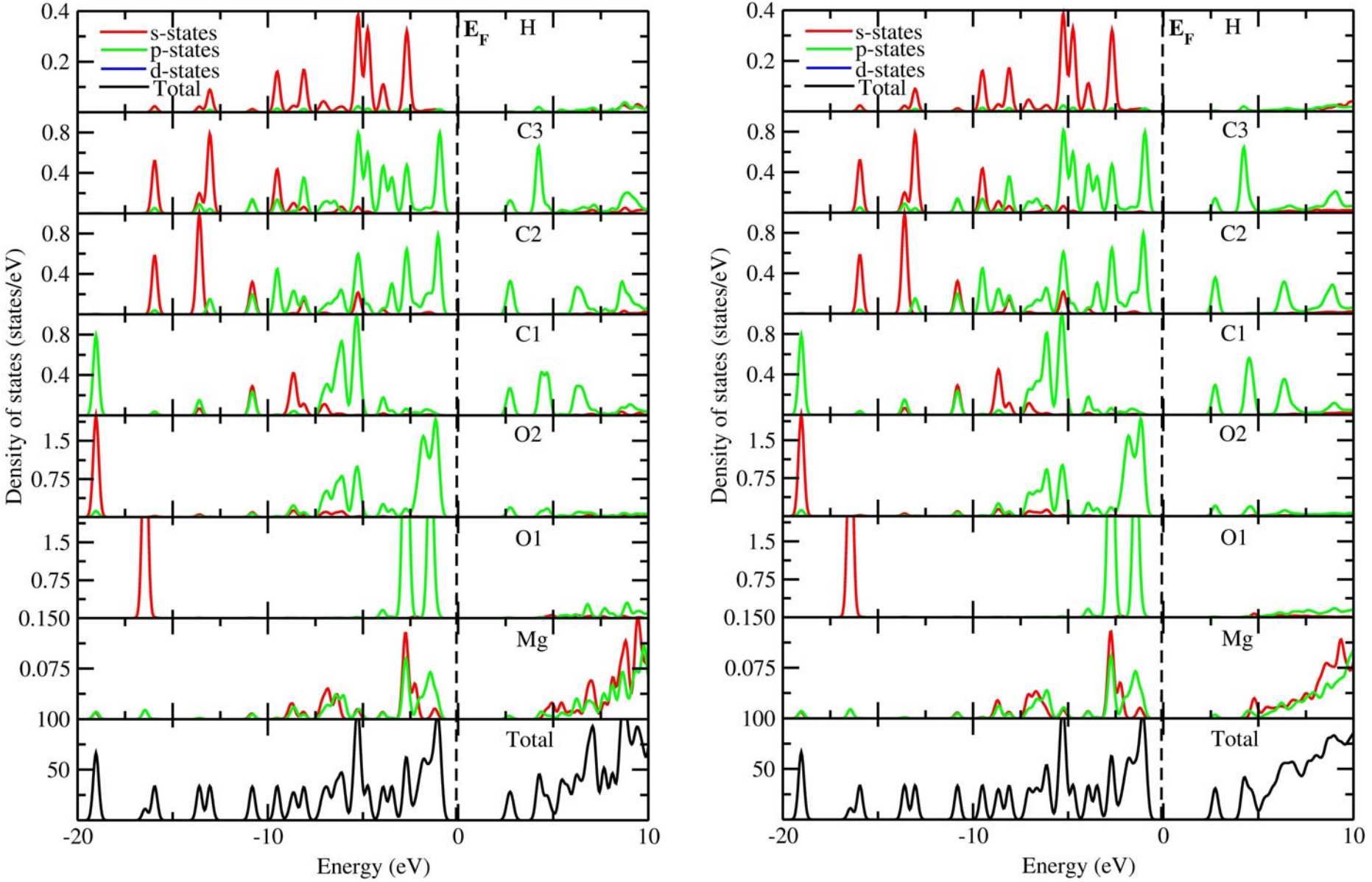

Figure S1. Calculated partial density of states (PDOS) for Mg-IRMOF-1 obtained from (a) **Γ** point (1×1×1) only **k**-mesh and (b) 3×3×3 **k**-mesh using the Monkhorst–Pack scheme.

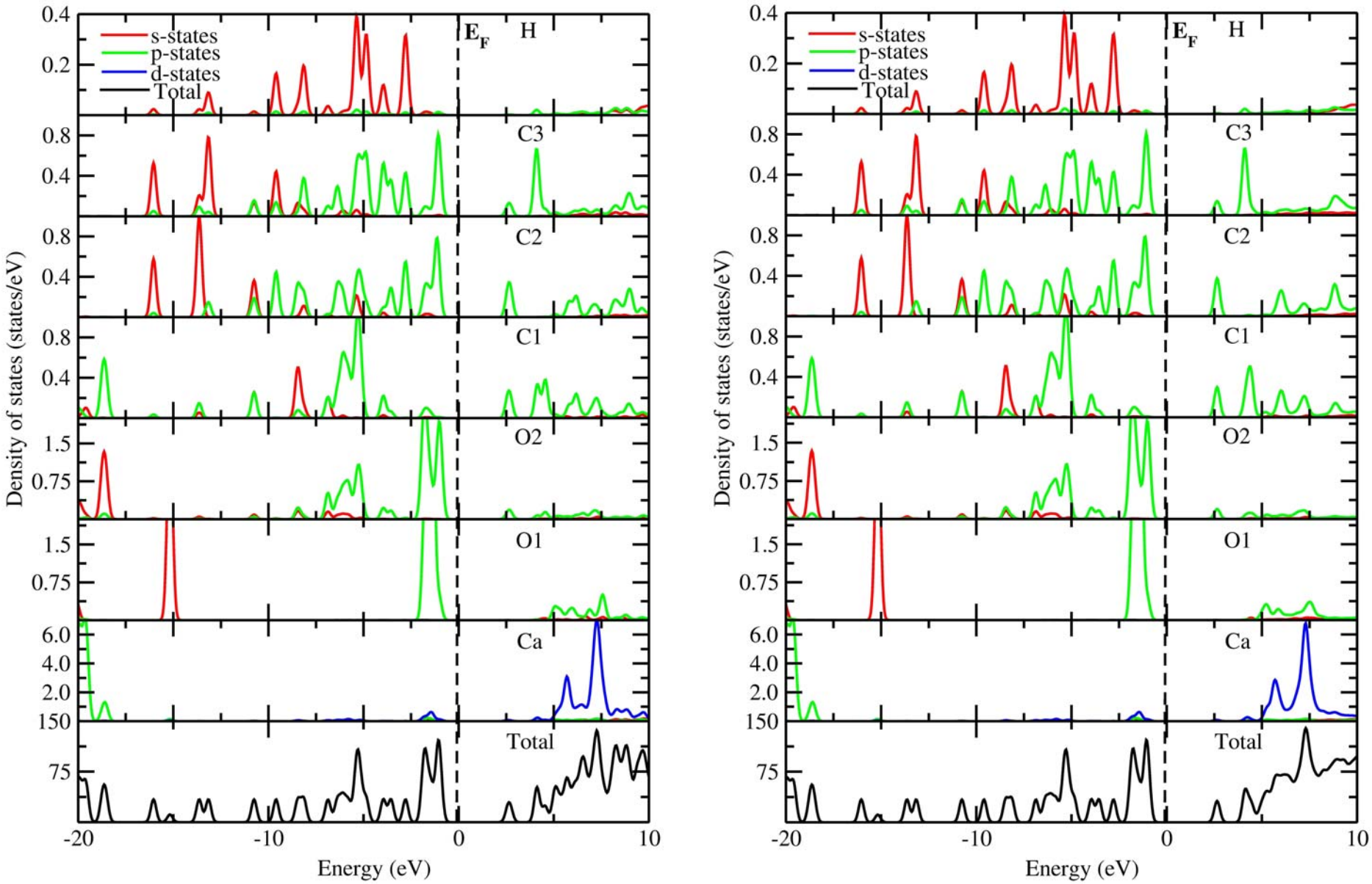

Figure S2. Calculated partial density of states (PDOS) for Ca-IRMOF-1 obtained from (a) **Γ** point (1×1×1) only **k**-mesh and (b) 3×3×3 **k**-mesh using the Monkhorst–Pack scheme.

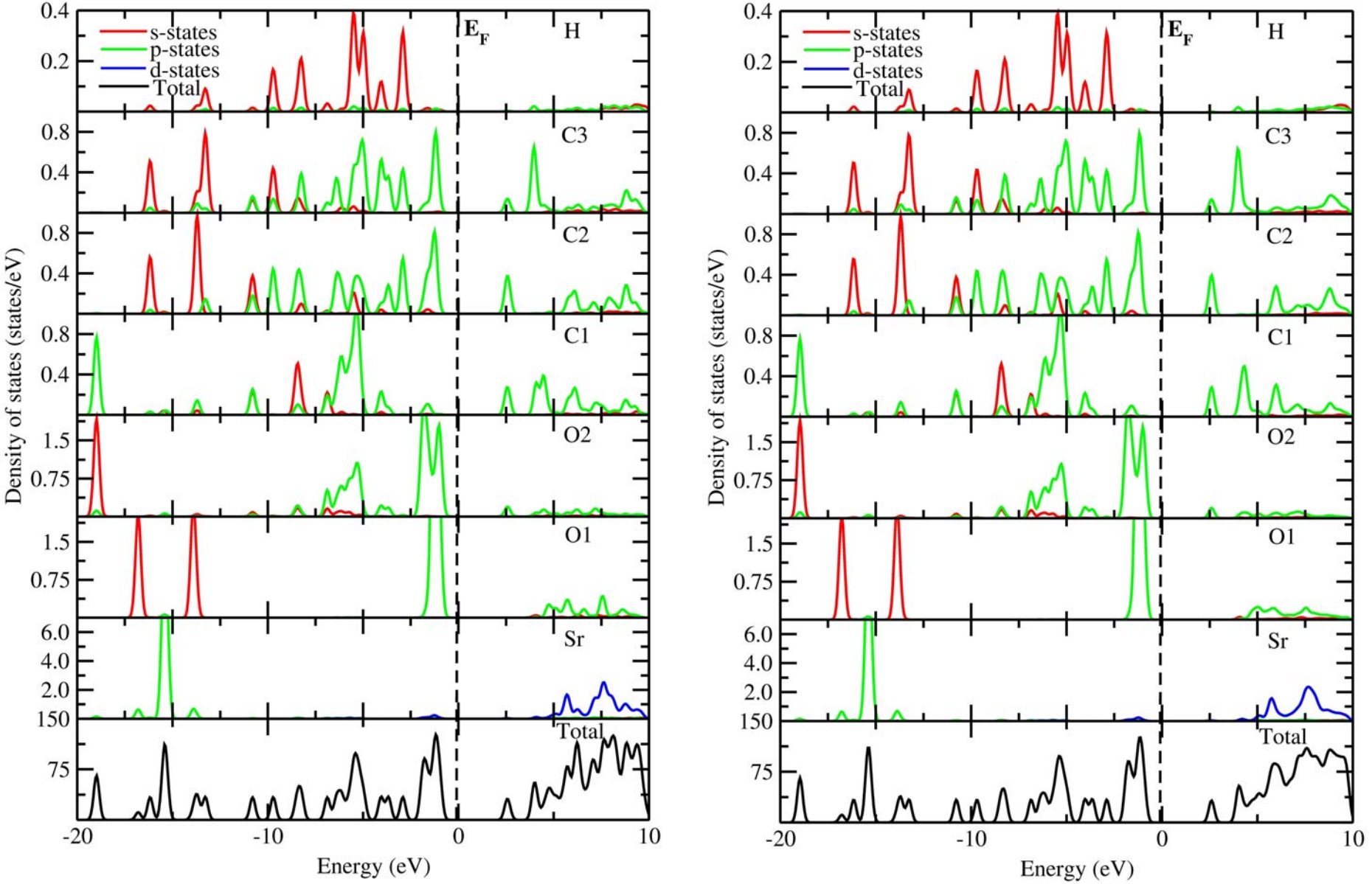

Figure S3. Calculated partial density of states (PDOS) for Sr-IRMOF-1 obtained from (a) **Γ** point (1×1×1) only **k**-mesh and (b) 3×3×3 **k**-mesh using the Monkhorst–Pack scheme.

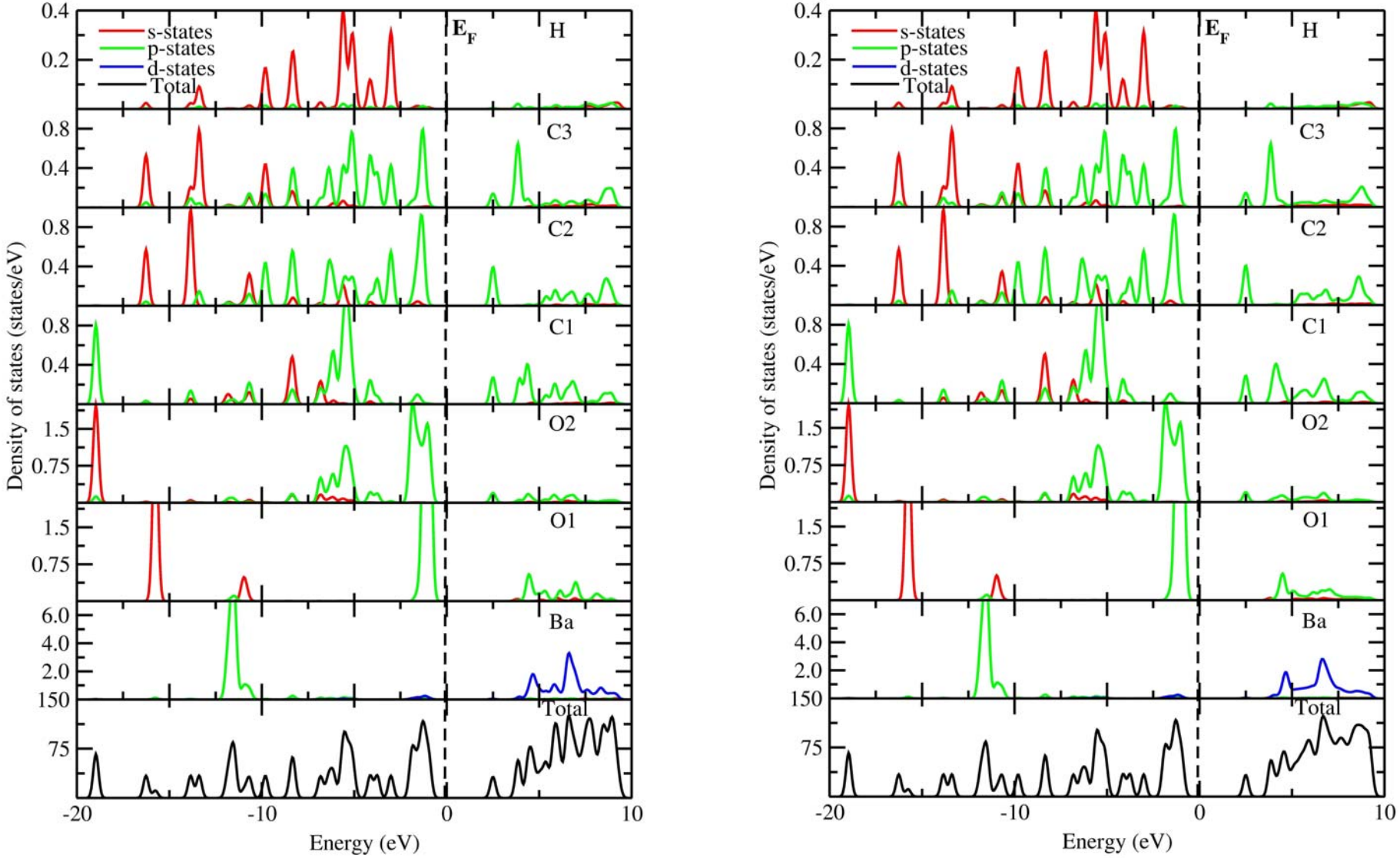

Figure S4. Calculated partial density of states (PDOS) for Ba-IRMOF-1 obtained from (a) **Γ** point (1×1×1) only **k**-mesh and (b) 3×3×3 **k**-mesh using the Monkhorst–Pack scheme.

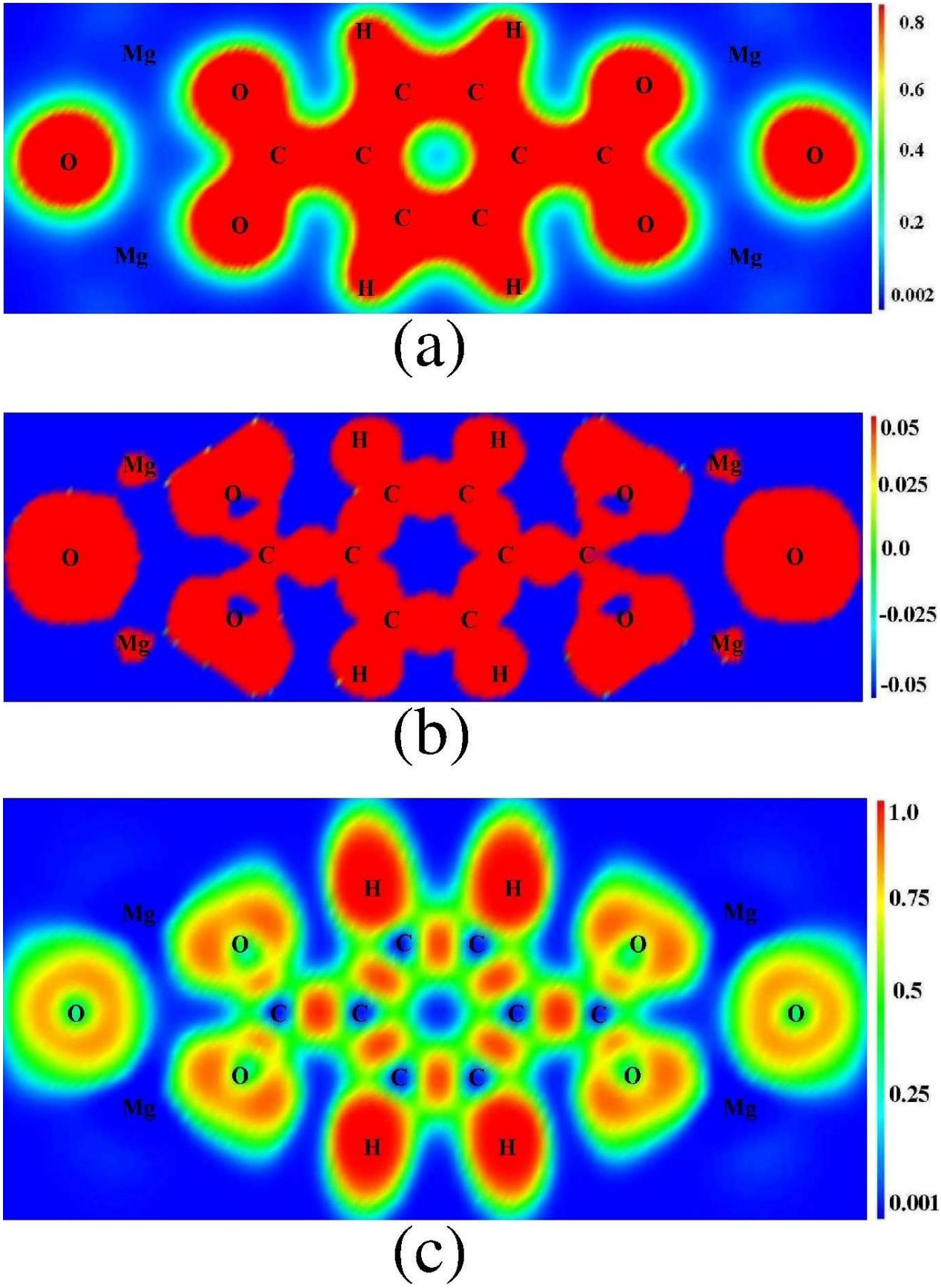

Figure S5. Calculated charge density (a), charge transfer (b), and electron localization function, ELF (c) plots for Mg-IRMOF-1 in the (110) plane.

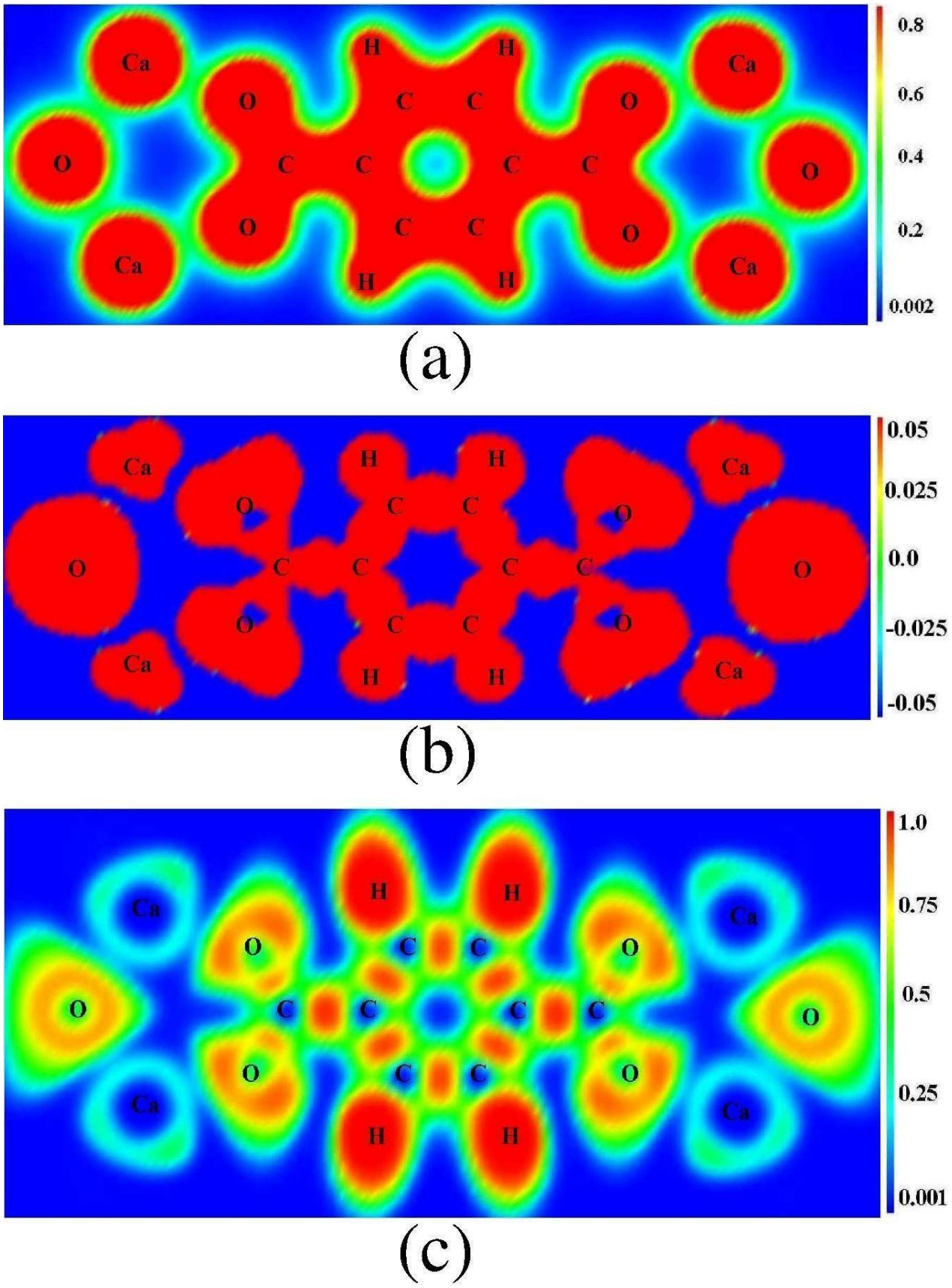

Figure S6. Calculated charge density (a), charge transfer (b), and electron localization function, ELF (c) plots for Ca-IRMOF-1 in the (110) plane.

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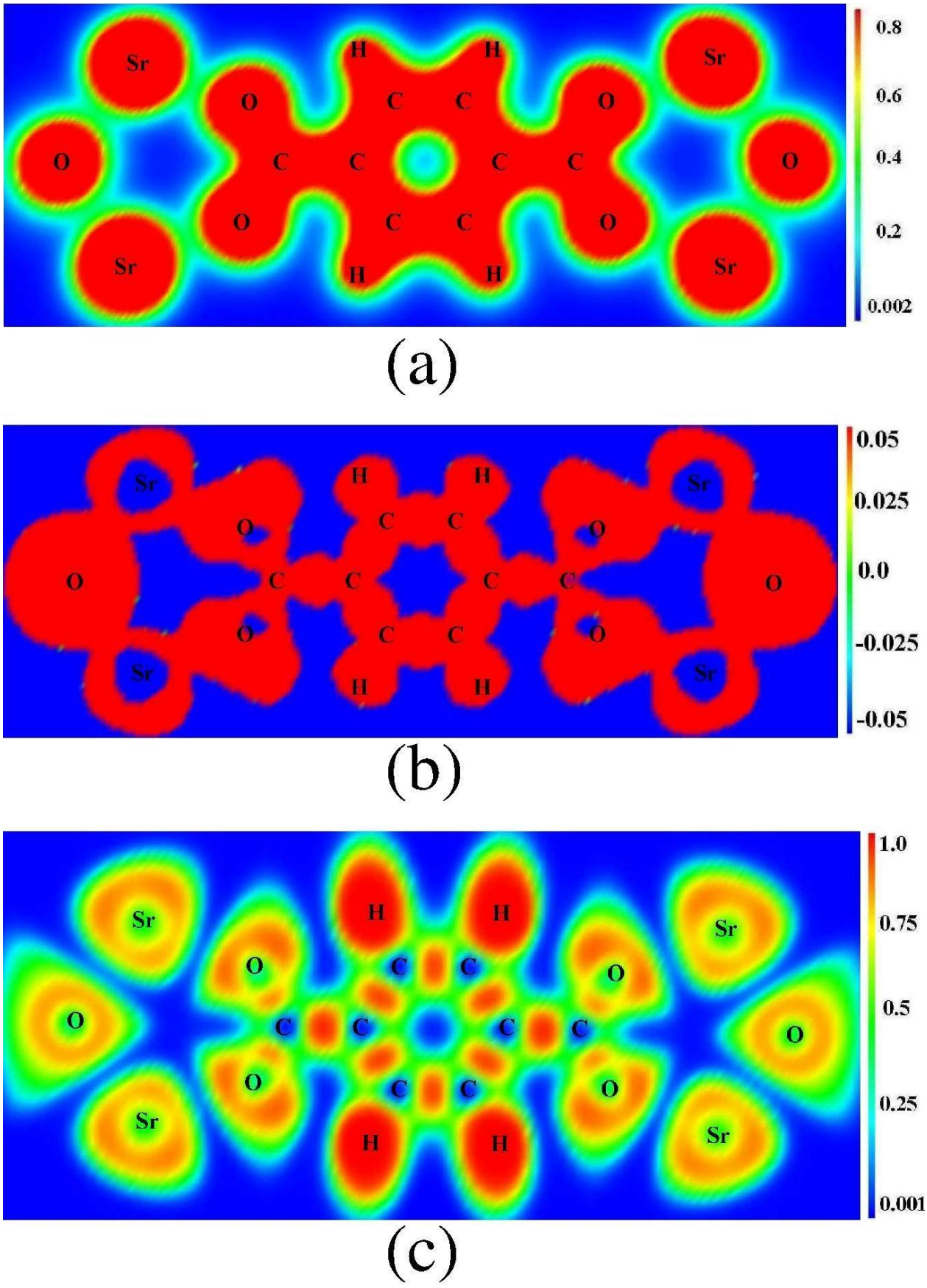
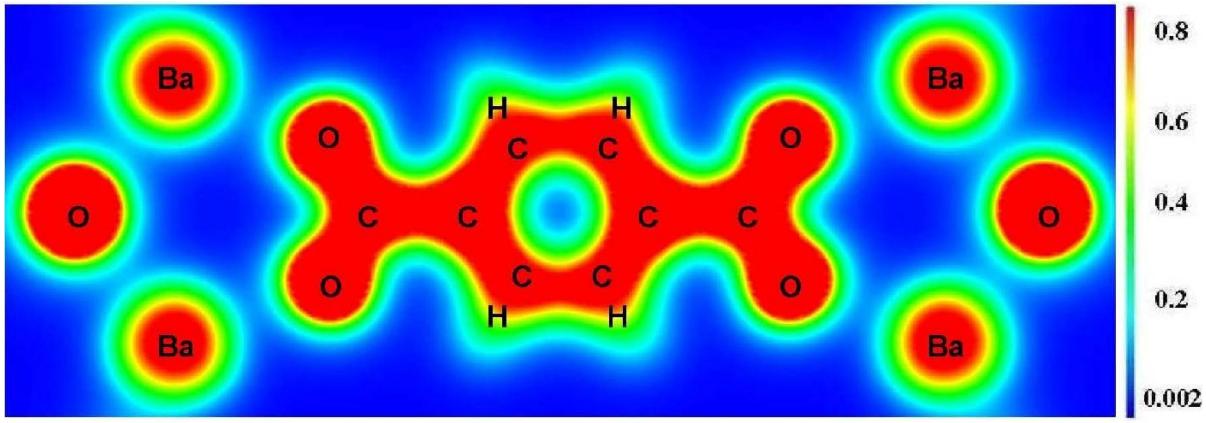
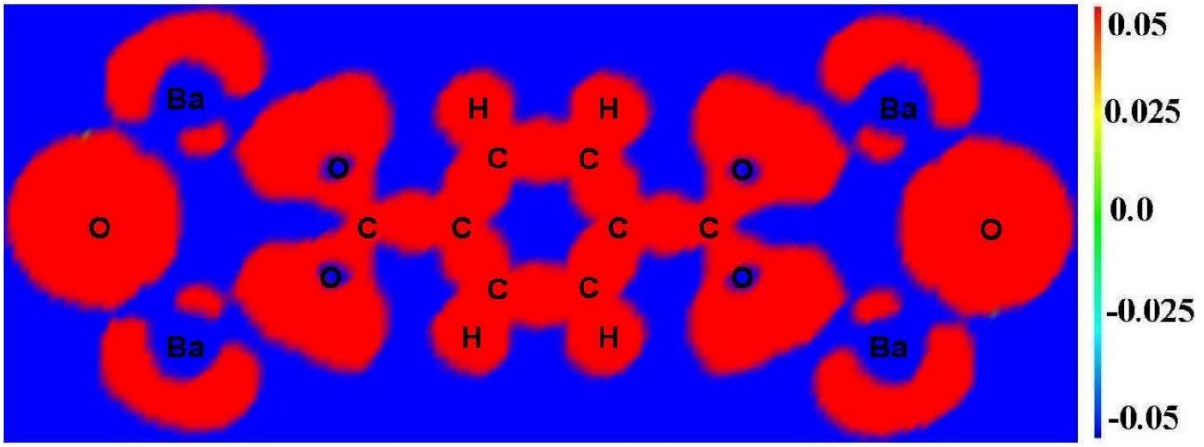


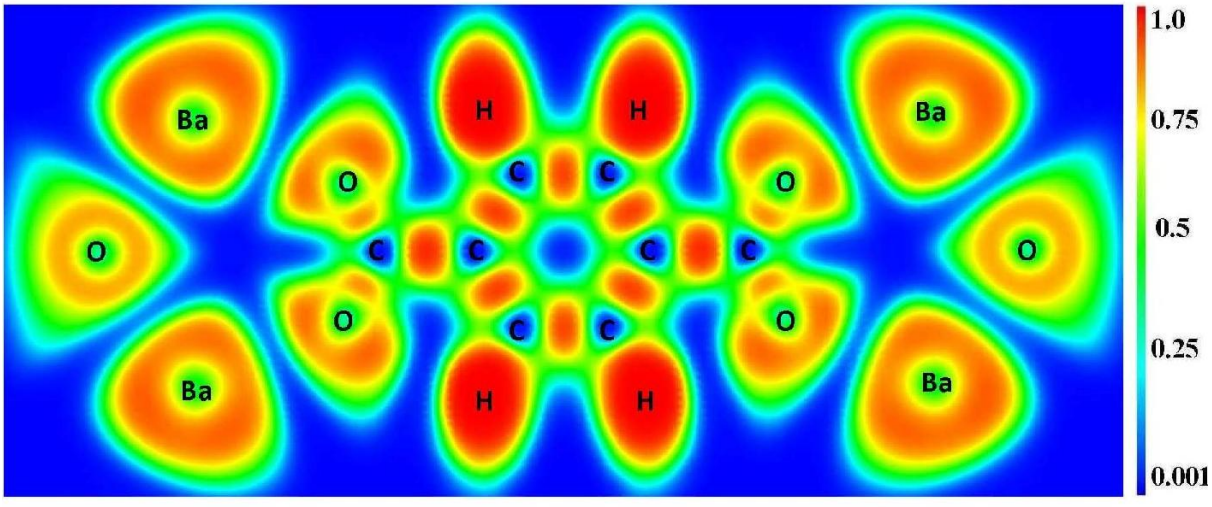
Figure S7. Calculated charge density (a), charge transfer (b), and electron localization function, ELF (c) plots for Sr-IRMOF-1 in the (110) plane.



(a)



(b)



(c)

Figure S8. Calculated charge density (a), charge transfer (b), and electron localization function, ELF (c) plots for Ba-IRMOF-1 in the (110) plane.

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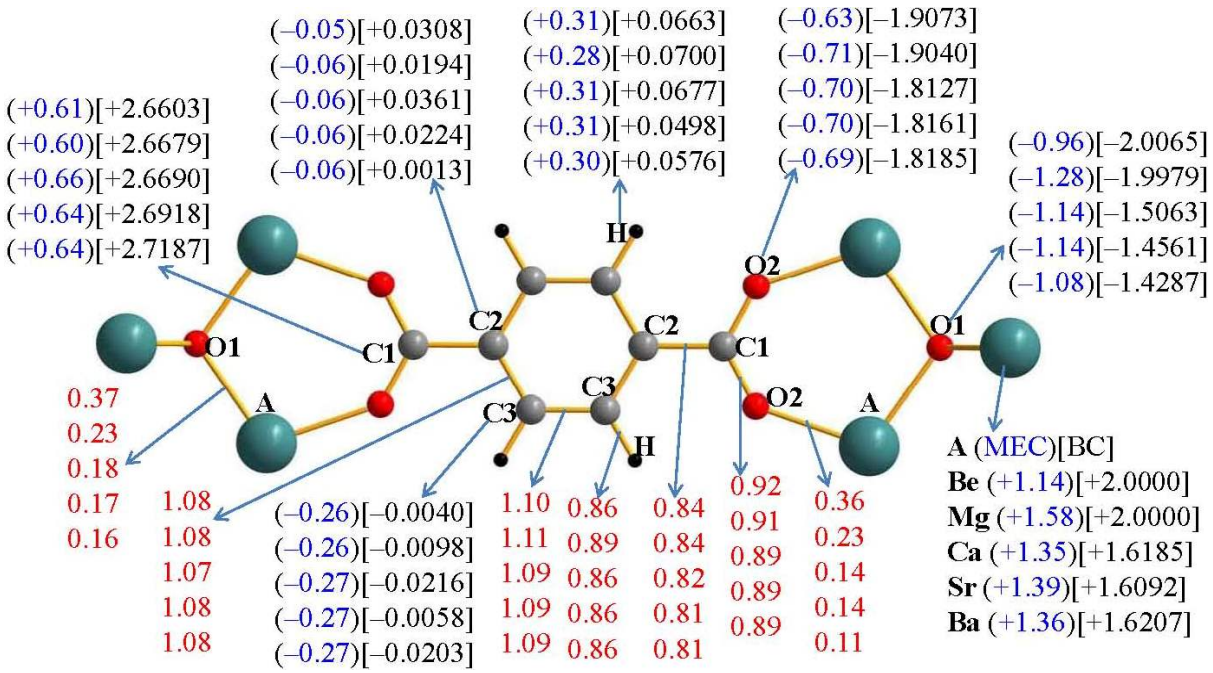

Figure S9. Calculated Bader charges (BC; black color in brackets), bond overlap populations (BOP; red color) and Mulliken effective charges (MEC; blue color in parentheses) for the *A*-IRMOF-1 series (*A* = Be, Mg, Ca, Sr, Ba).

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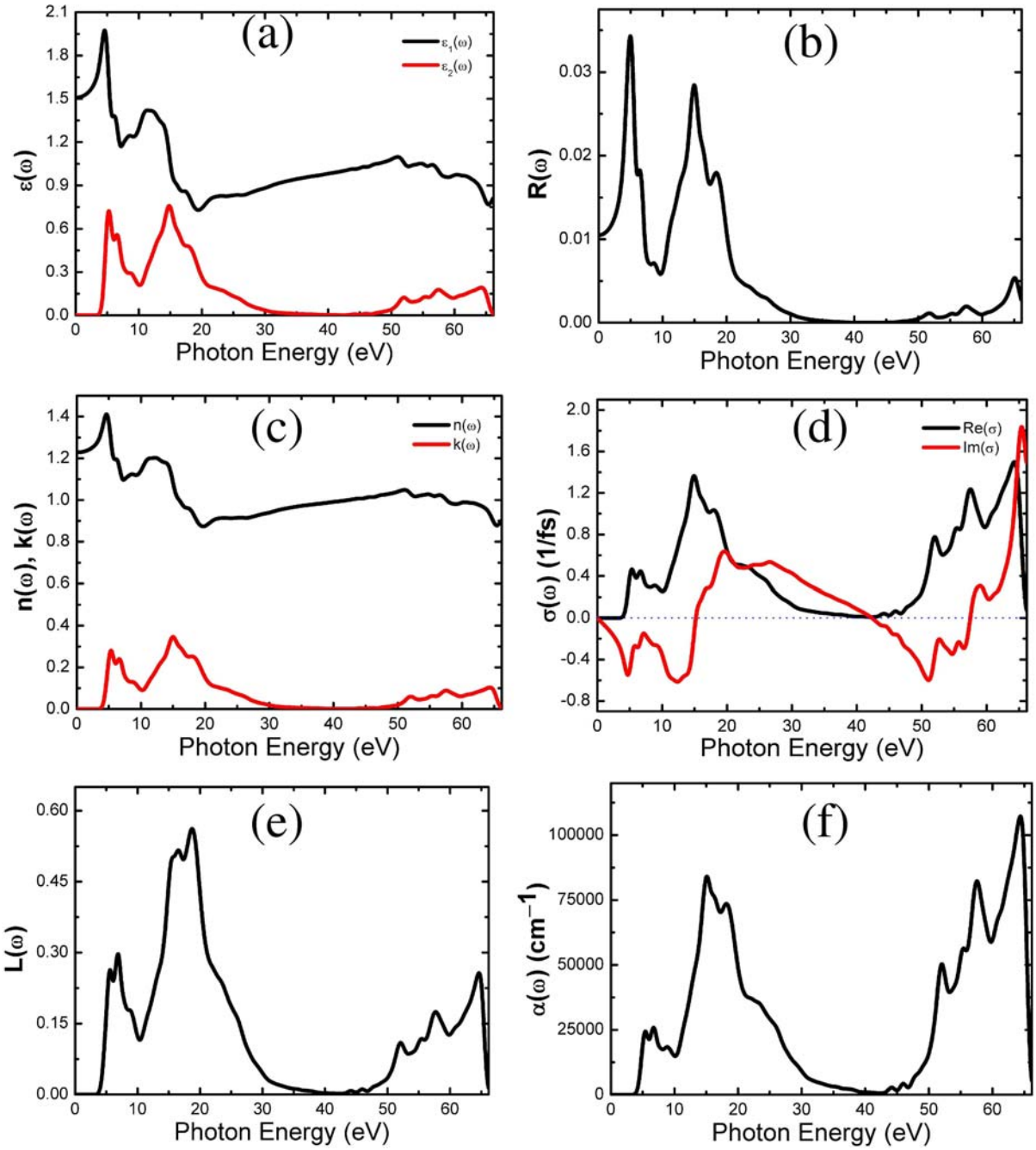

Figure S10. Calculated optical properties for Mg-IRMOF-1: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), and (f) absorption α(ω).

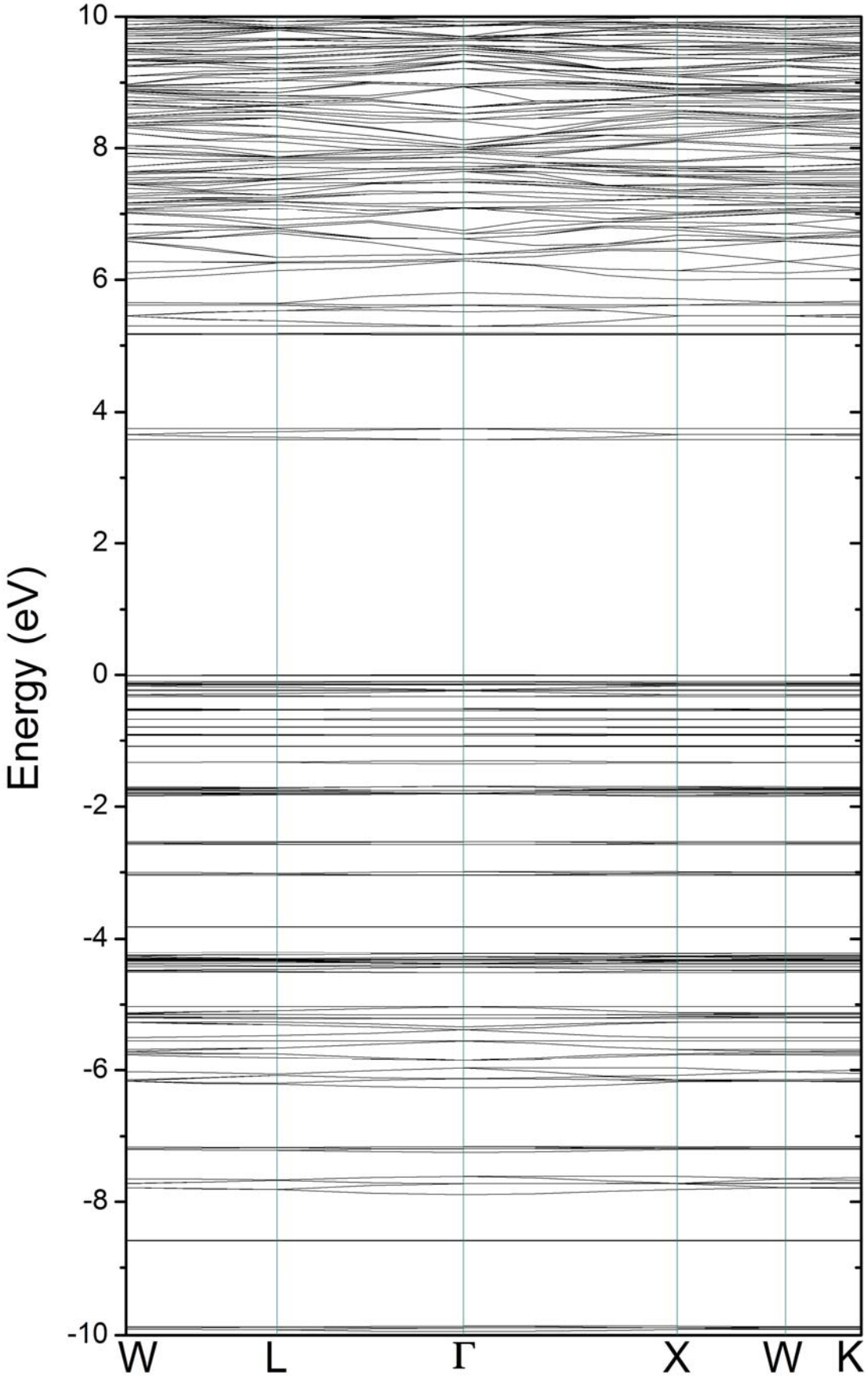

Figure S11. Band structure of Mg-IRMOF-1. The Fermi level is set to zero.

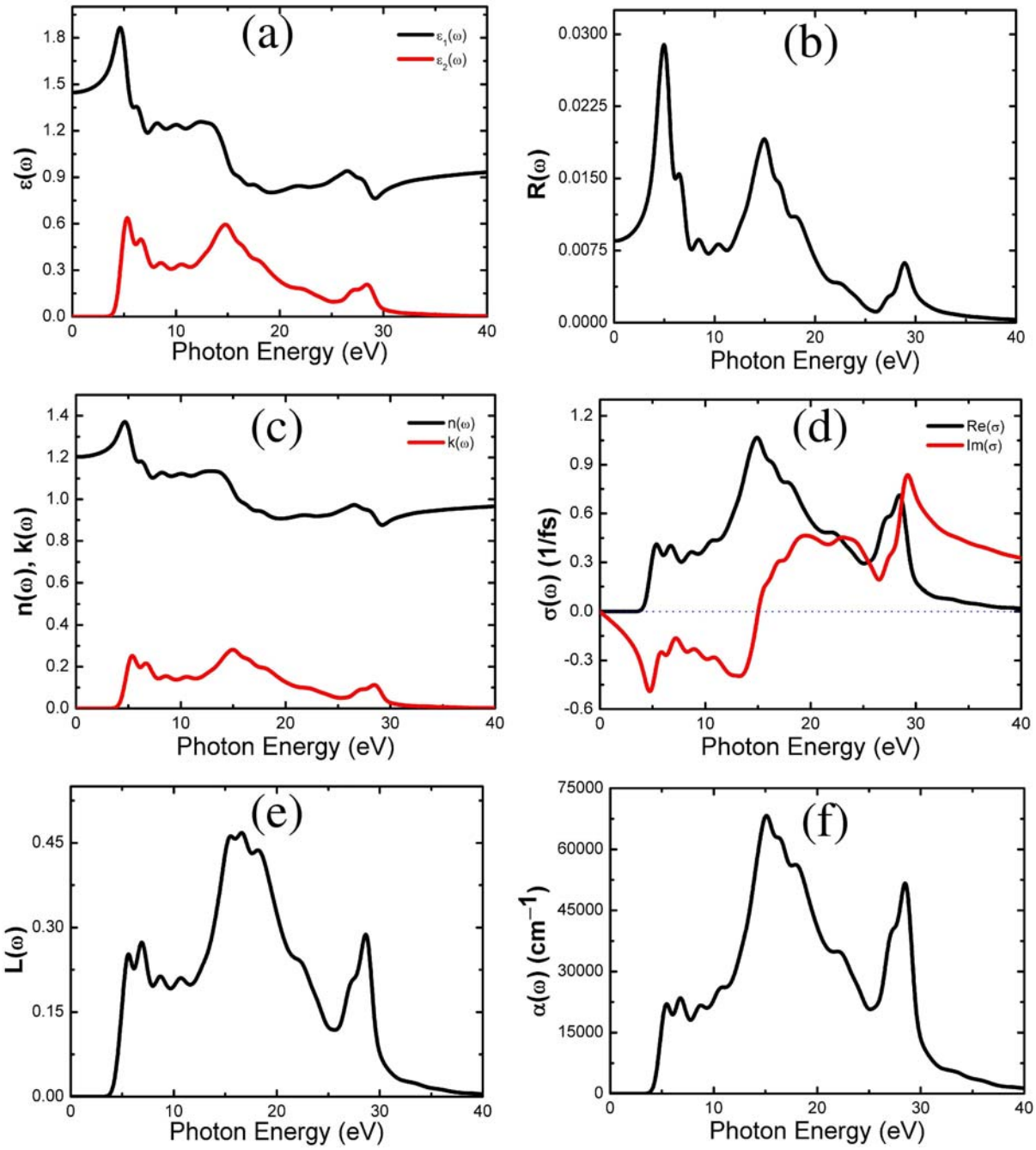

Figure S12. Calculated optical properties for Ca-IRMOF-1: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), and (f) absorption α(ω).

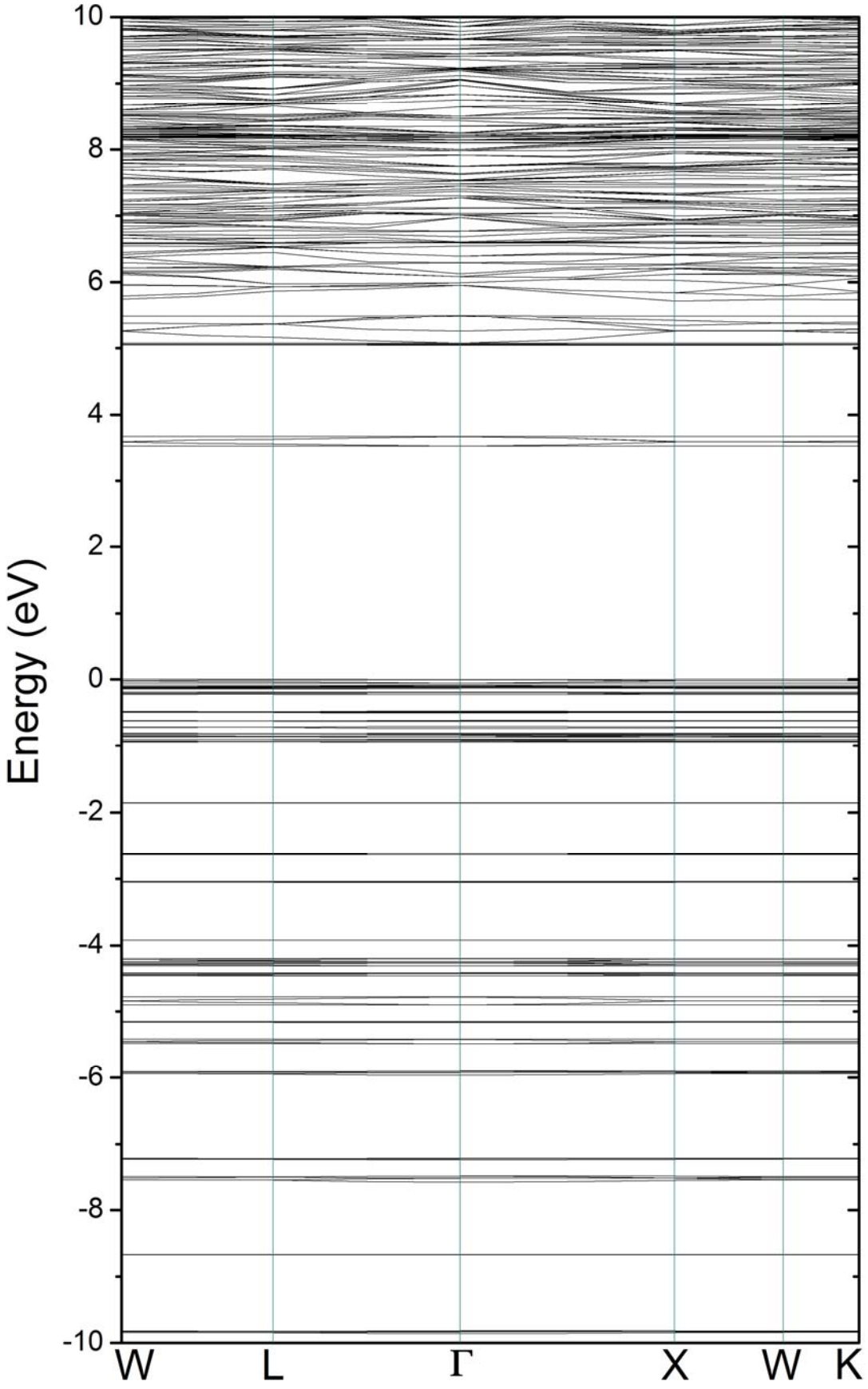

Figure S13. Band structure of Ca-IRMOF-1. The Fermi level is set to zero.

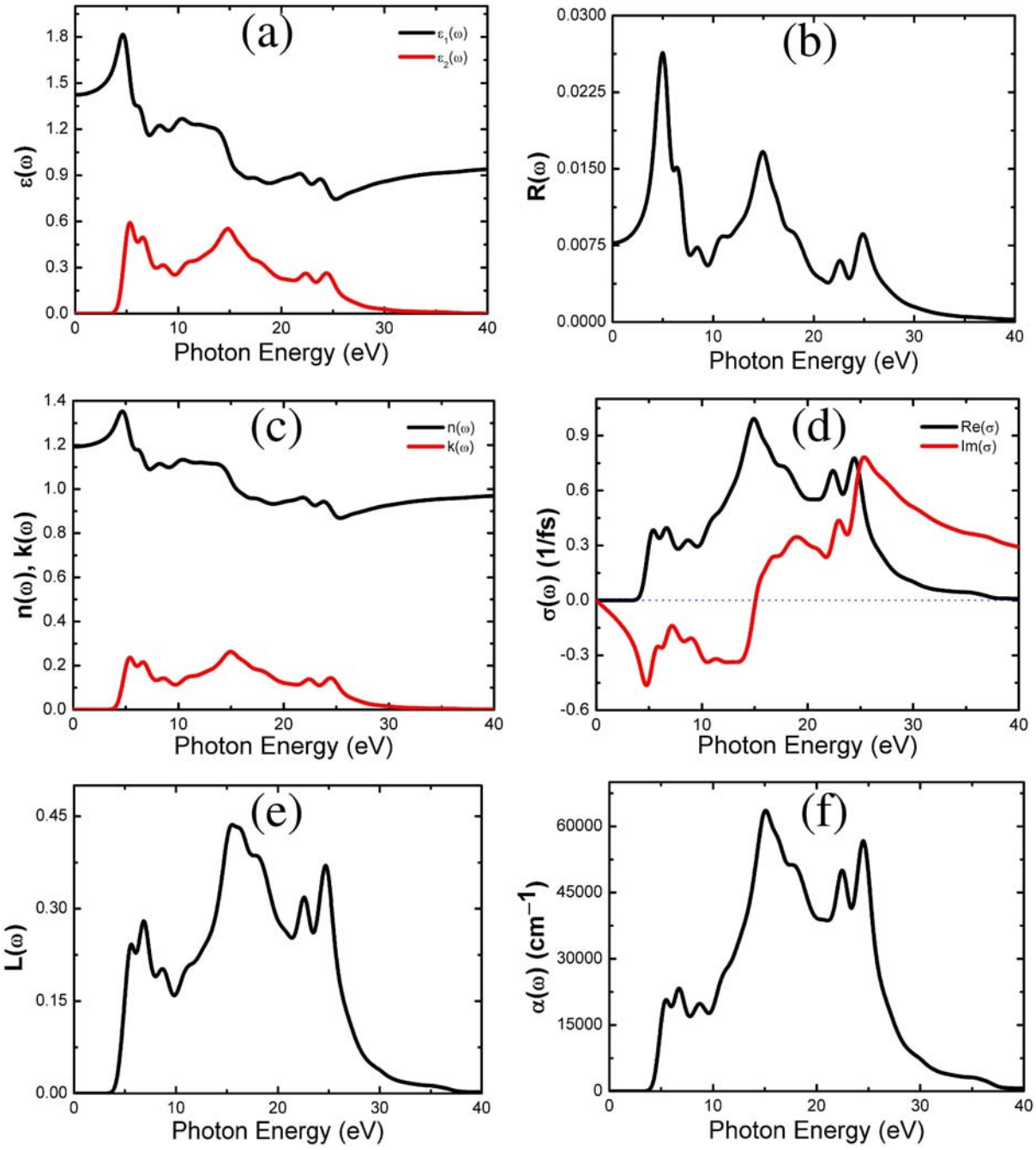

Figure S14. Calculated optical properties for Sr-IRMOF-1: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), and (f) absorption α(ω).

Supplementary Material (ESI) for PCCP

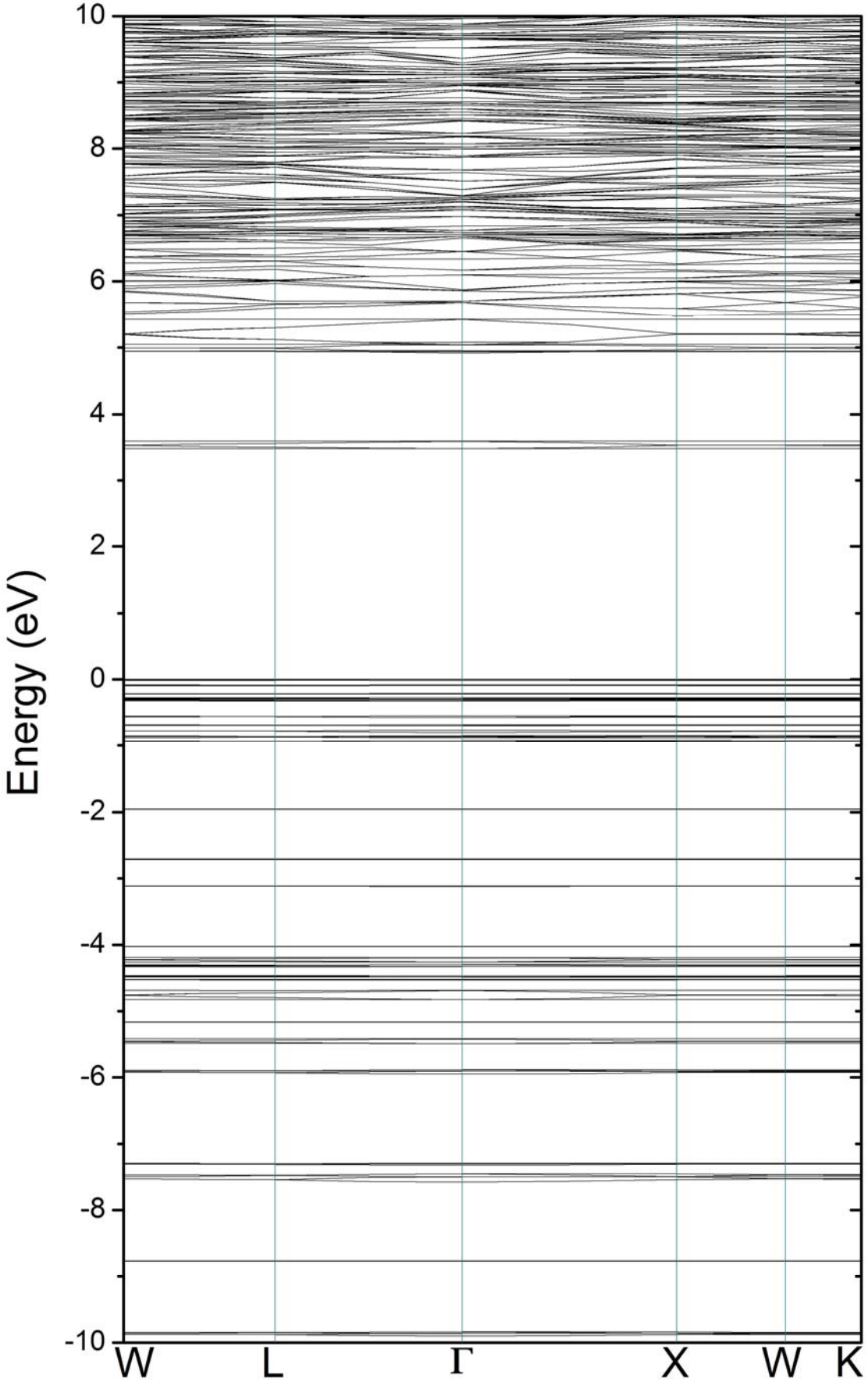

Figure S15. Band structure of Sr-IRMOF-1. The Fermi level is set to zero.

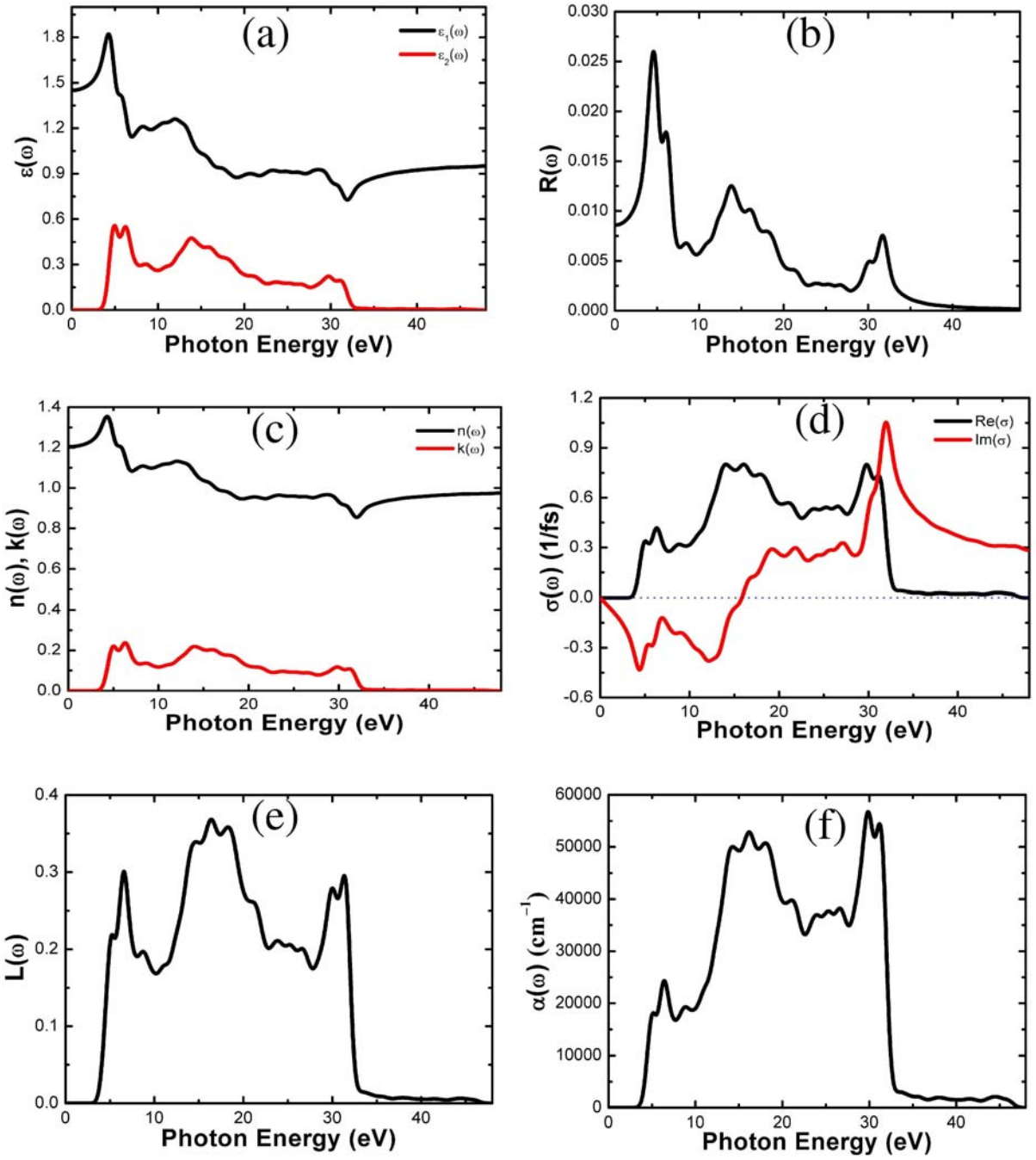

Figure S16. The calculated optical spectra for Ba-IRMOF-1: (a) dielectric function ε(ω); (b) reflectivity R(ω); (c) refractive index **n**(ω) and extinction coefficient **k**(ω); (d) optical conductivity σ(ω); (e) energy loss function L(ω); (f) absorption coefficient α(ω) (cm^{-1}).

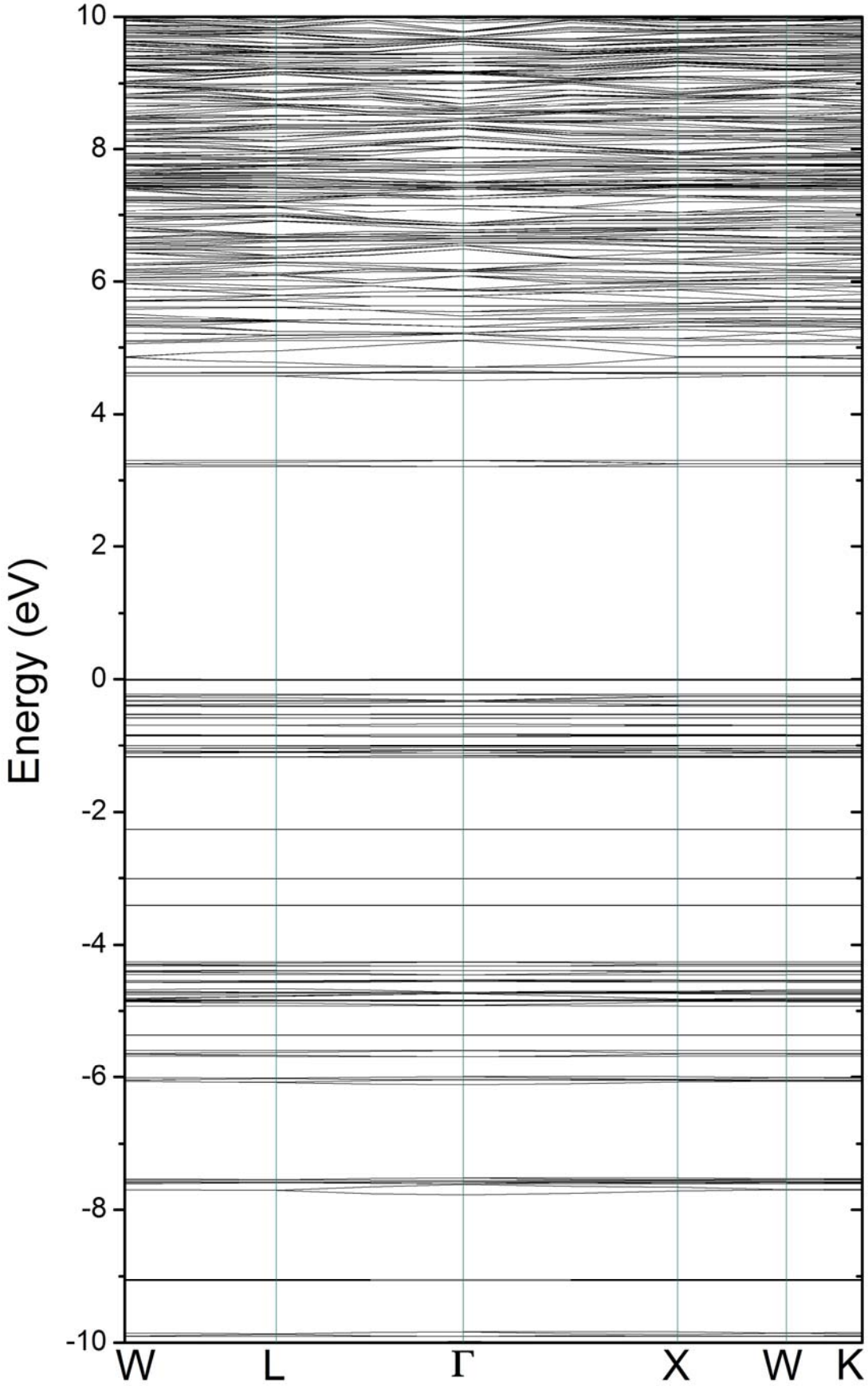

Figure S17. The calculated electronic band structure of Ba-IRMOF-1. The Fermi level is set to zero and placed in the valence band maximum.