

***Ab initio* investigations on the crystal structure, formation enthalpy, electronic structure, chemical bonding, and optical properties of experimentally synthesized isorecticular metal-organic framework-10 and its analogues: *M*-IRMOF-10 (*M* = Zn, Cd, Be, Mg, Ca, Sr and Ba)**

***Supporting Information***

Li-Ming Yang<sup>\*†</sup>, Ponniah Ravindran<sup>‡</sup>, Ponniah Vajeeston<sup>‡</sup>, and Mats Tilset<sup>\*†</sup>

<sup>†</sup>*Center of Theoretical and Computational Chemistry, Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, N-0315 Oslo, Norway,* <sup>‡</sup>*Center for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, N-0315 Oslo, Norway*

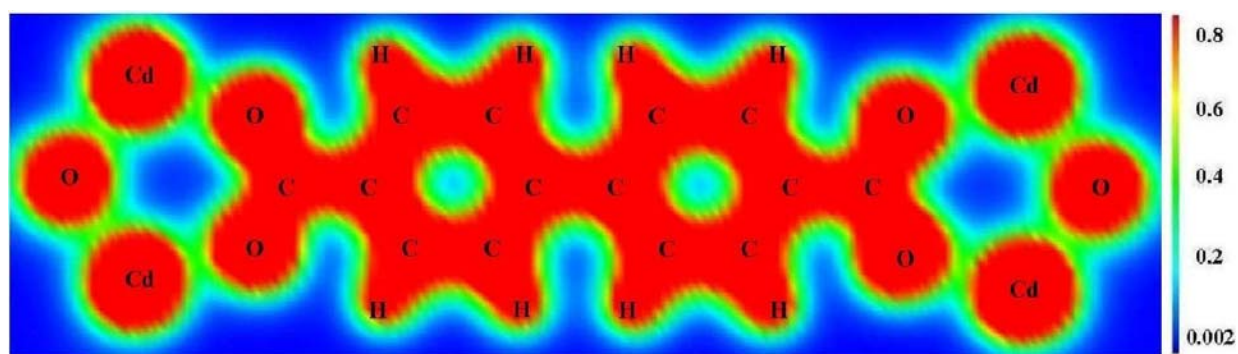
(E-mail of corresponding authors: [mats.tilset@kjemi.uio.no](mailto:mats.tilset@kjemi.uio.no) and [l.m.yang@kjemi.uio.no](mailto:l.m.yang@kjemi.uio.no); Fax: +47 22855441;)

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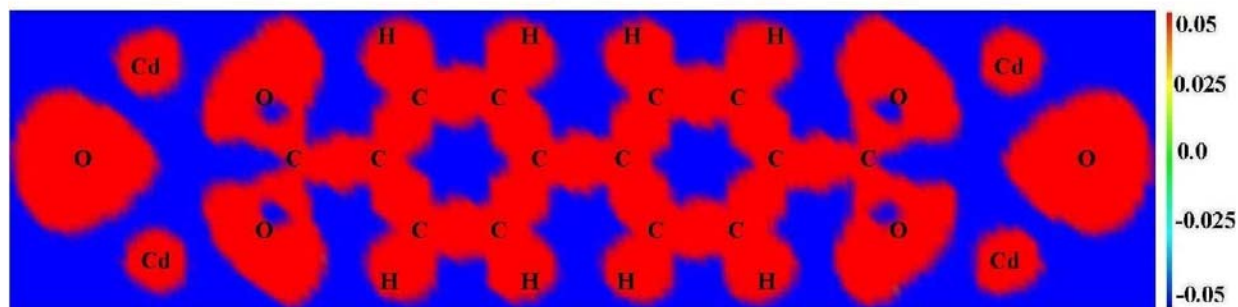
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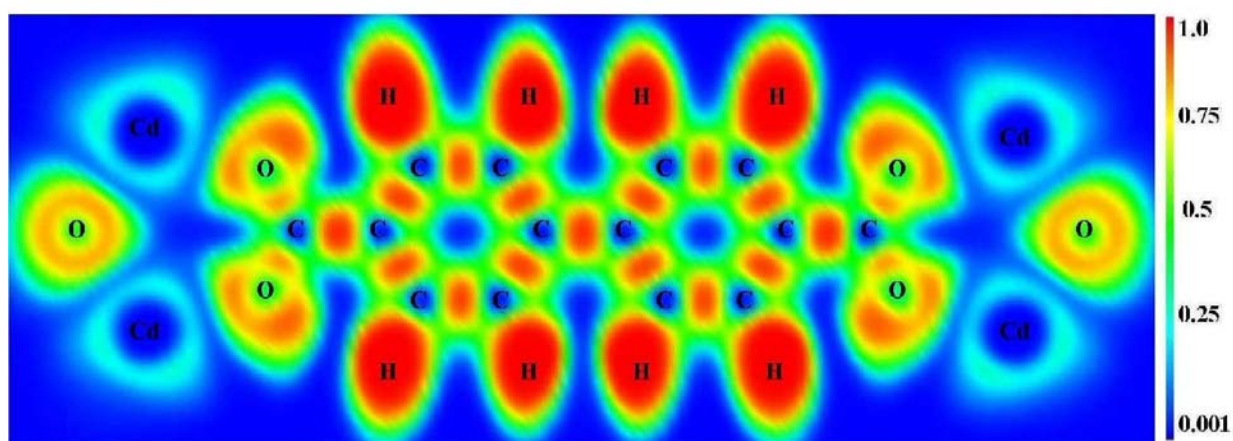
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(a)

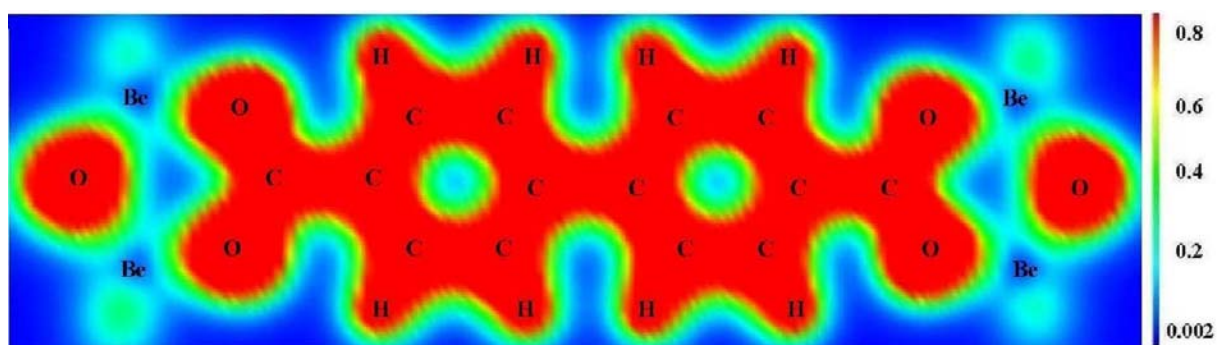


(b)

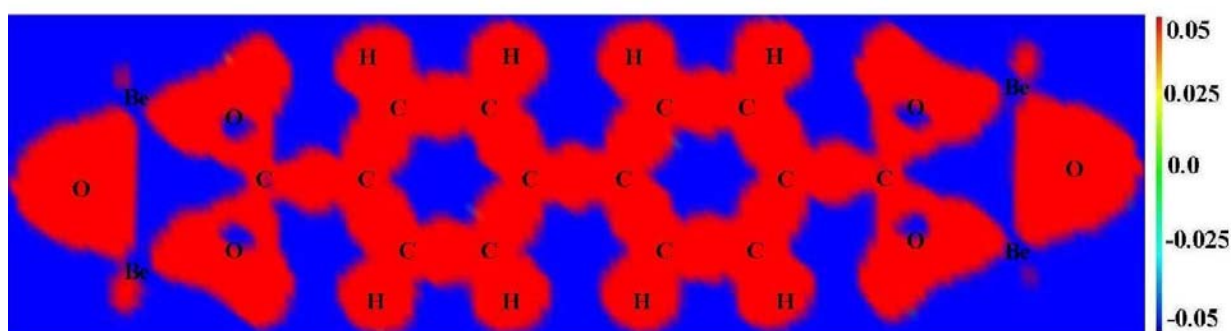


(c)

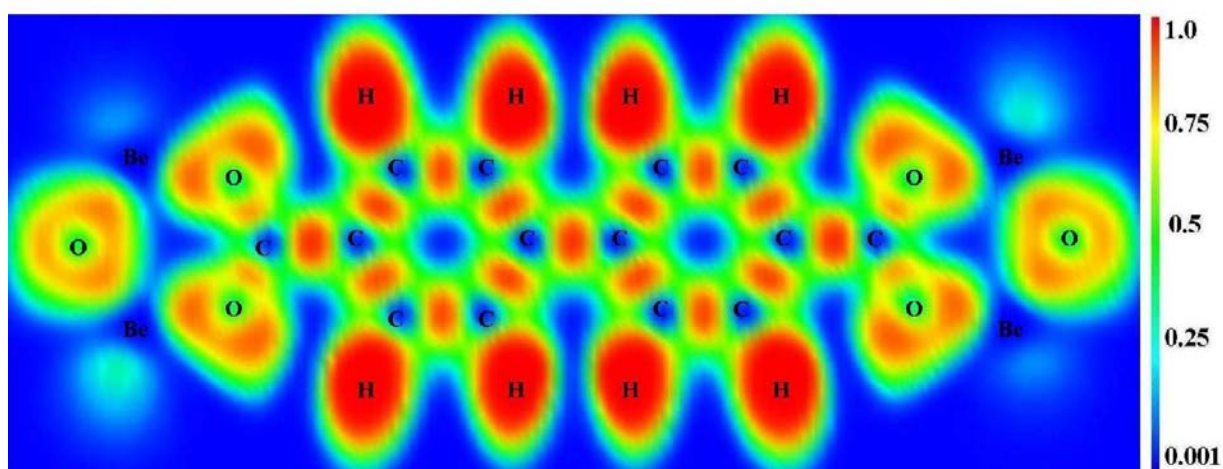
**Figure S1.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Cd-IRMOF-10 in the (110) plane.



(a)



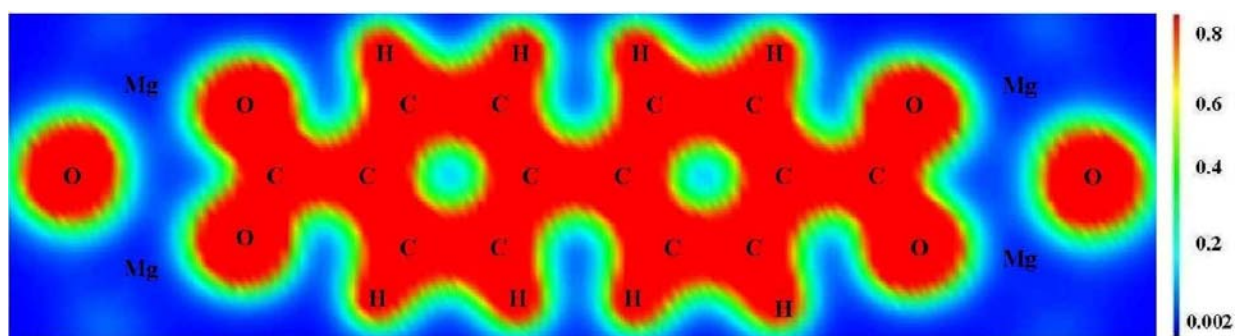
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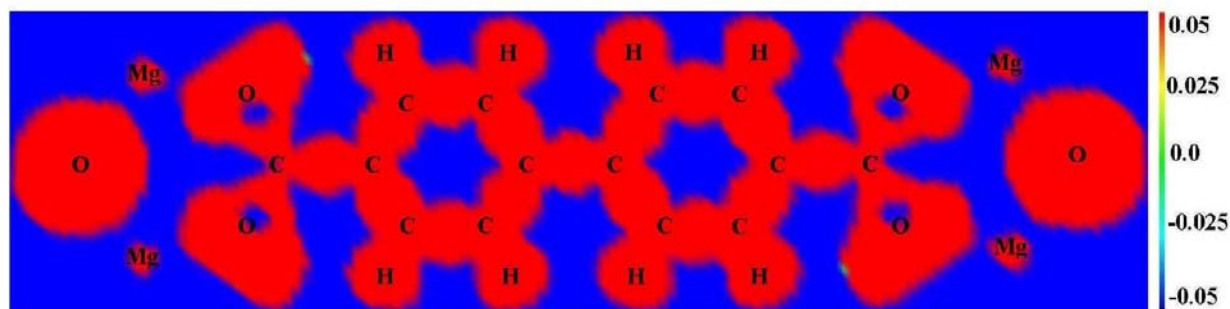
(c)

**Figure S2.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Be-IRMOF-10 in the (110) plane.

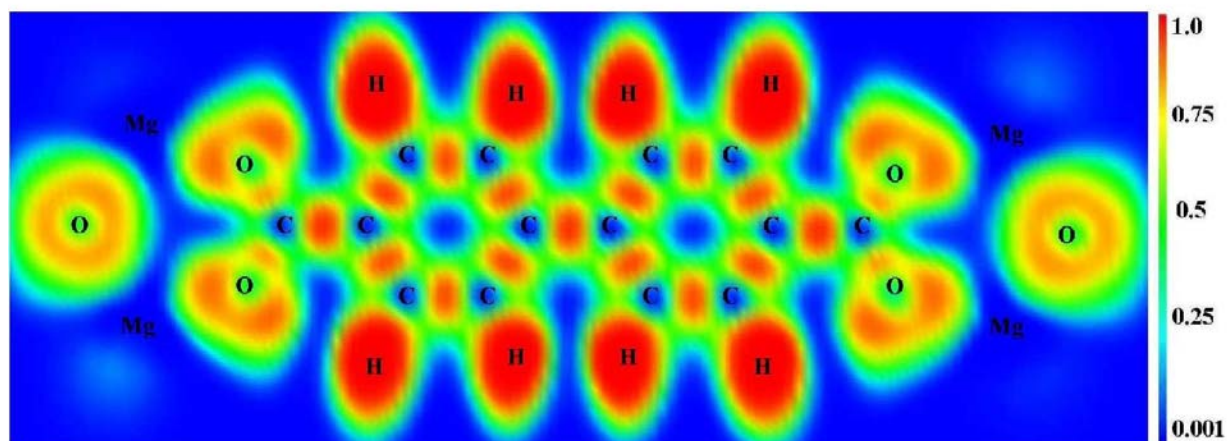




(a)



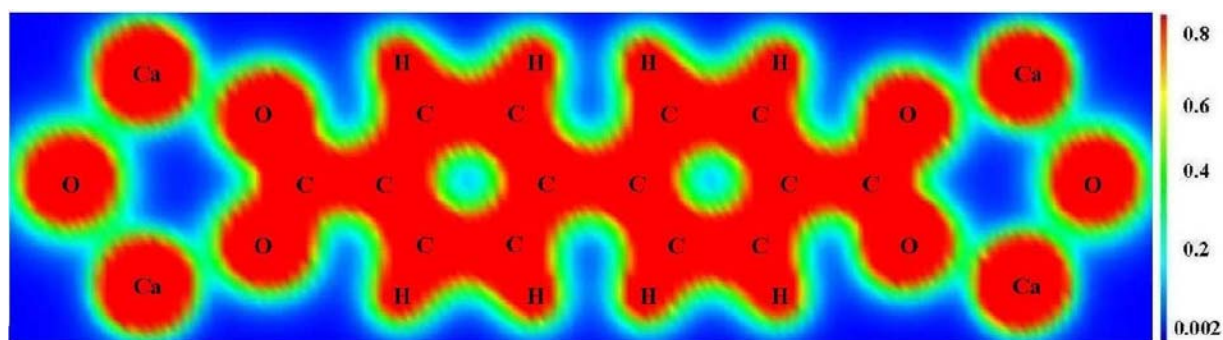
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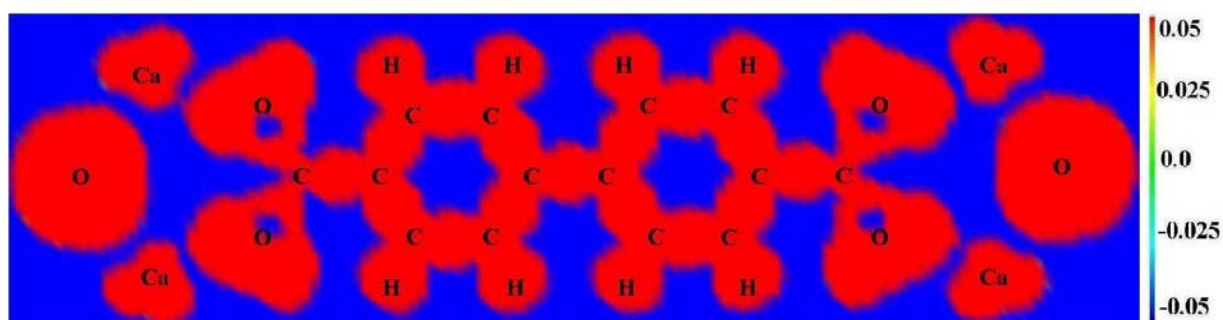
(c)

**Figure S3.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Mg-IRMOF-10 in the (110) plane.

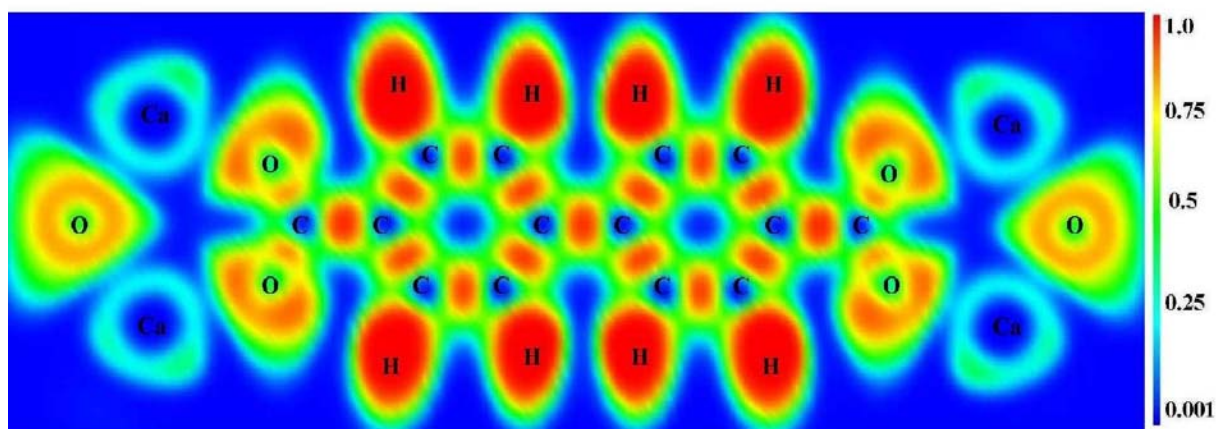




(a)

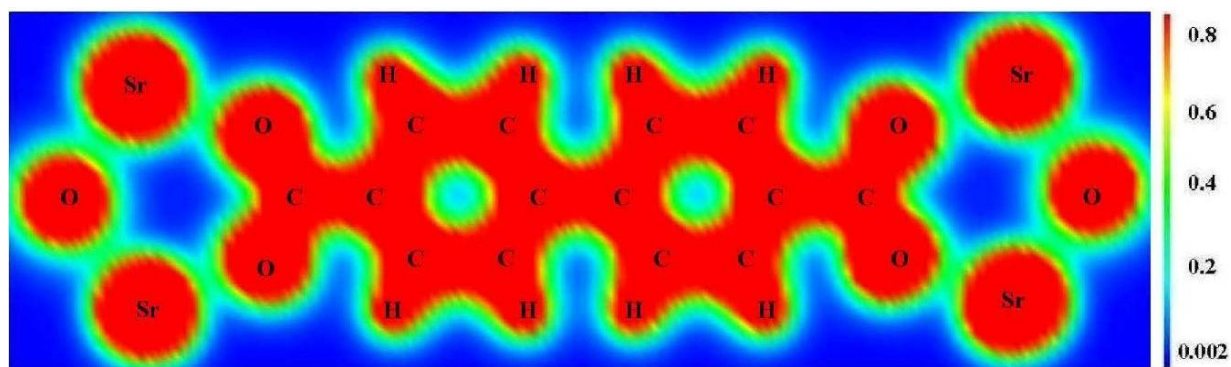


(b)

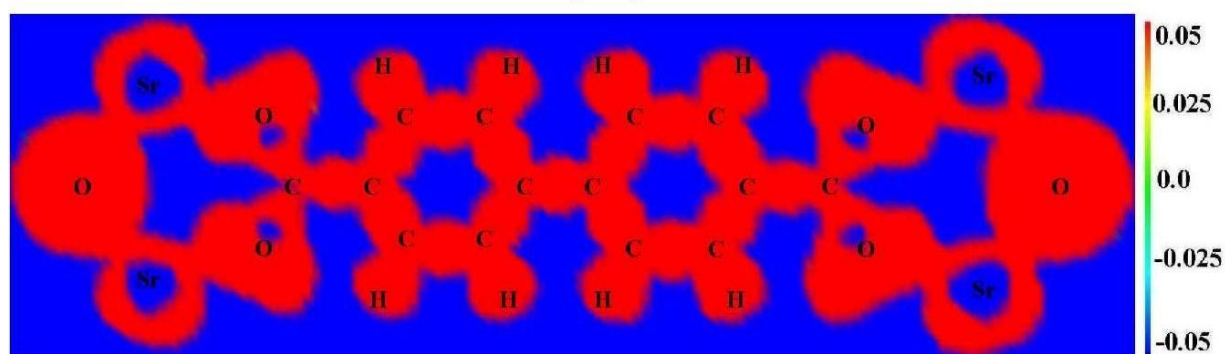


(c)

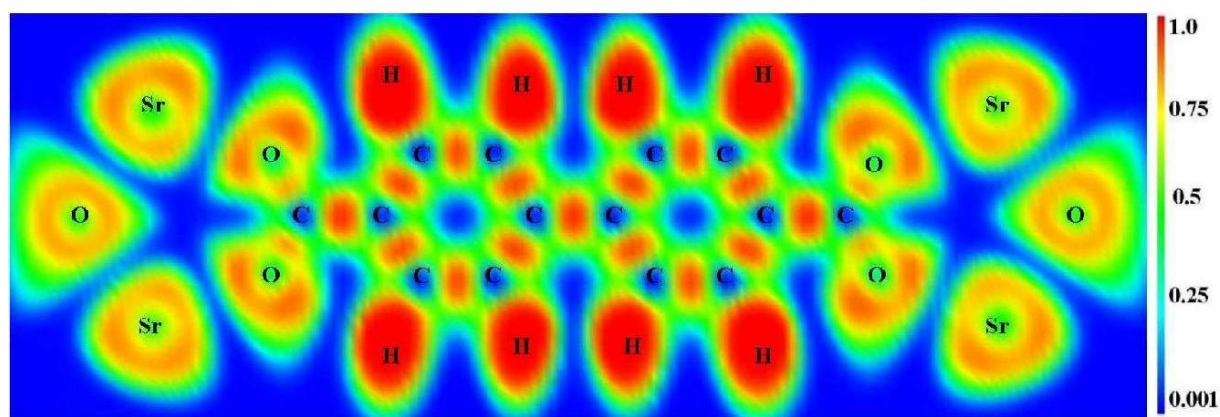
**Figure S4.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Ca-IRMOF-10 in the (110) plane.



(a)



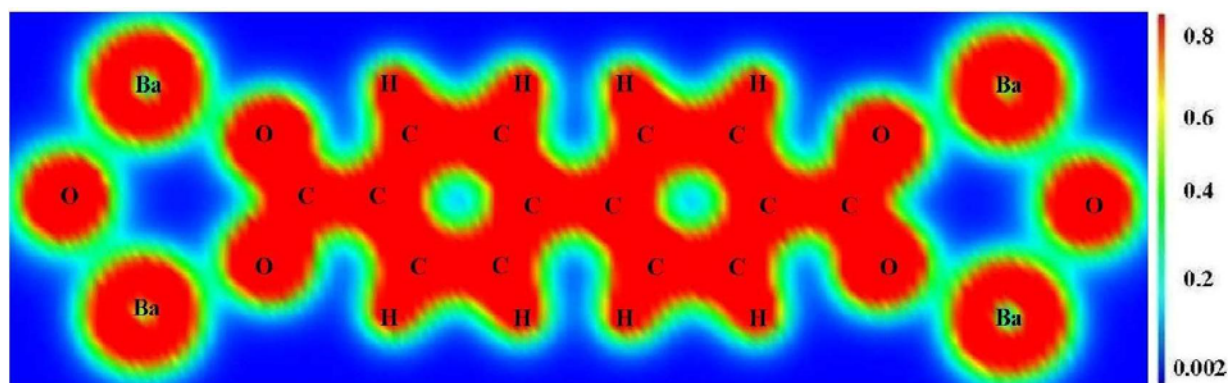
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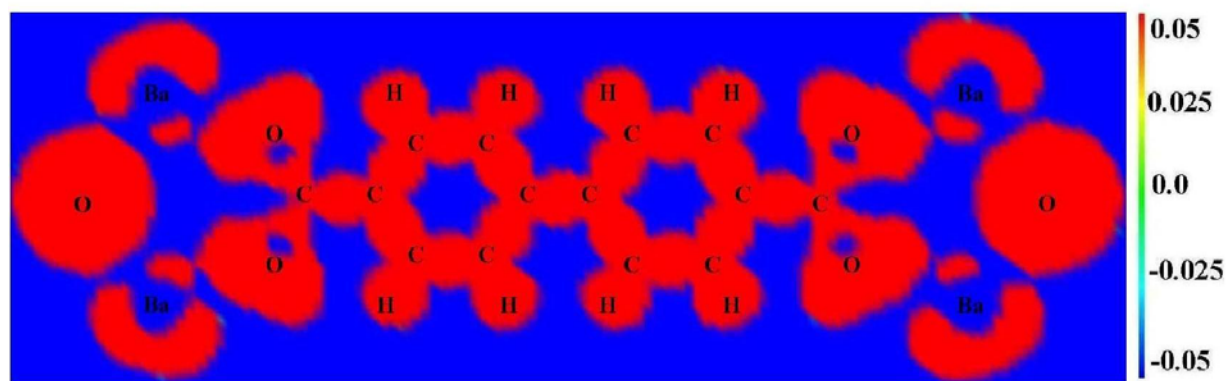
(c)

**Figure S5.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Sr-IRMOF-10 in the (110) plane.

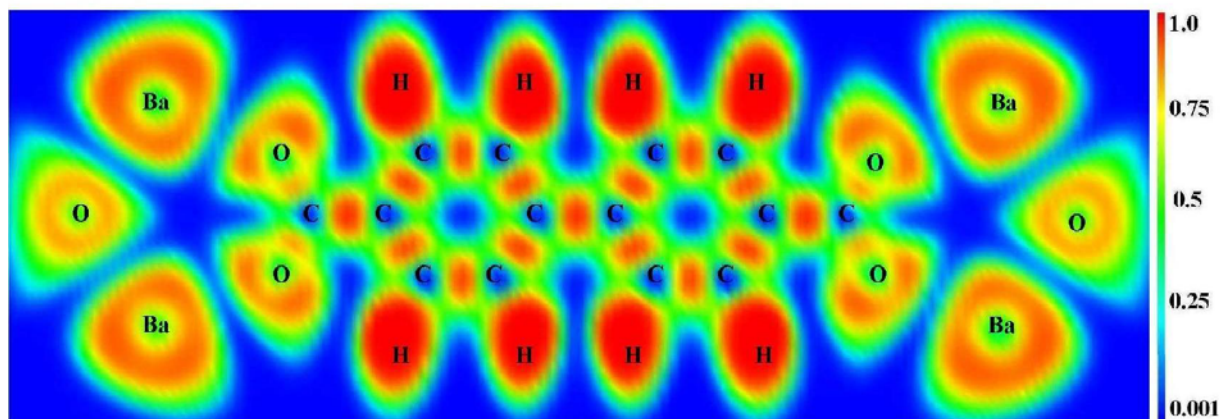




(a)



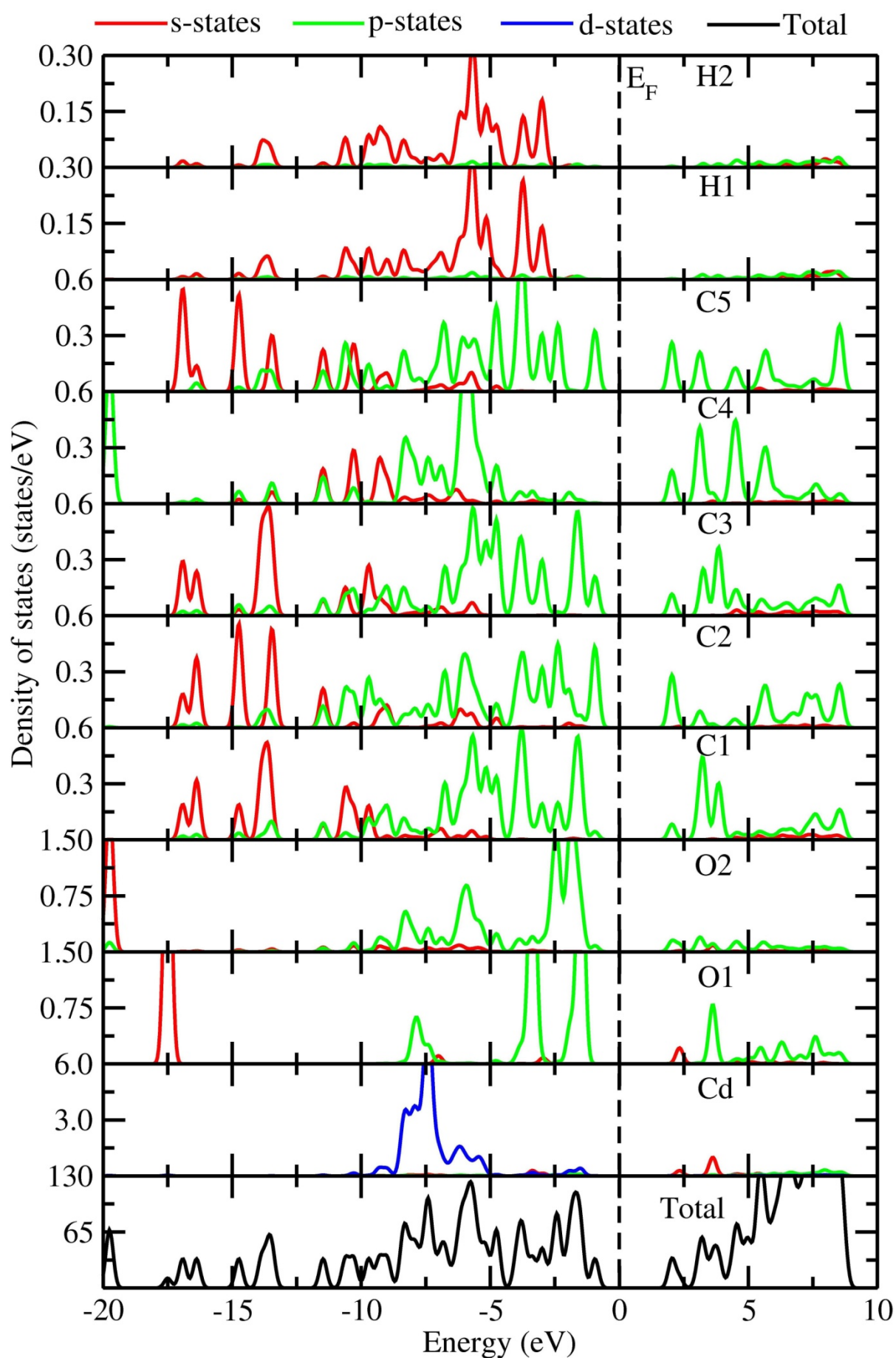
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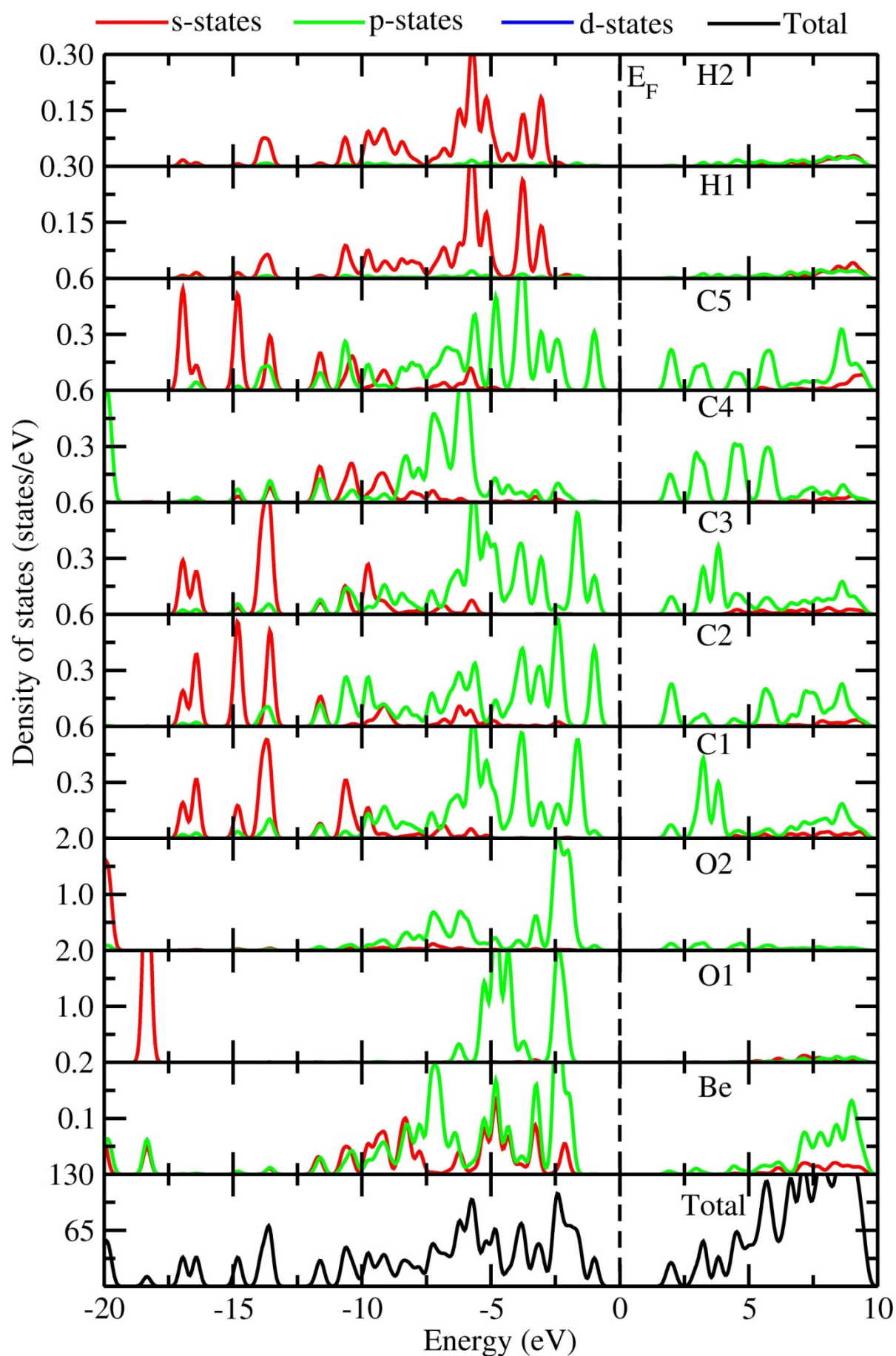
(c)

**Figure S6.** Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Ba-IRMOF-10 in the (110) plane.

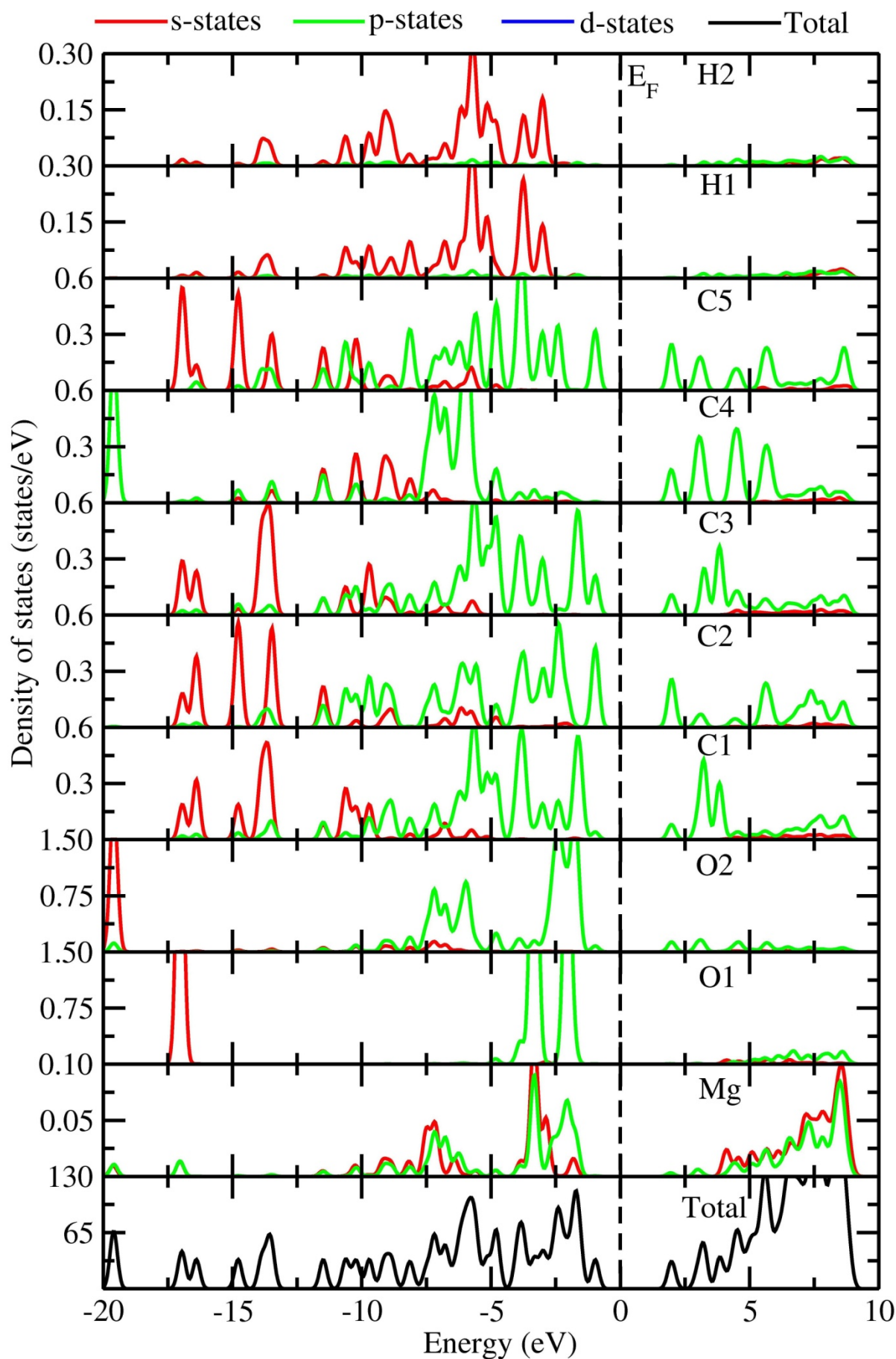




**Figure S7.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Cd-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

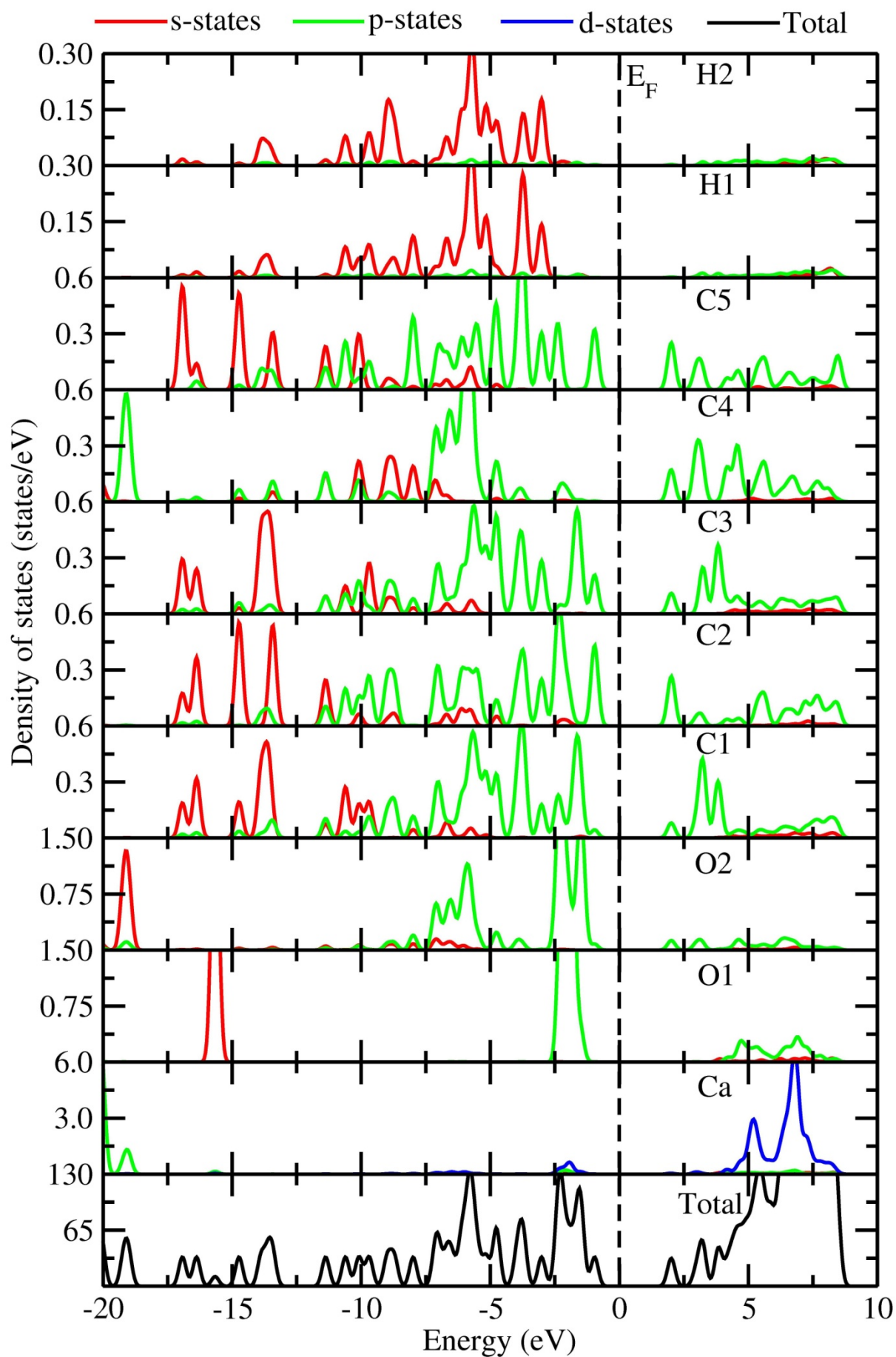


**Figure S8.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Be-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

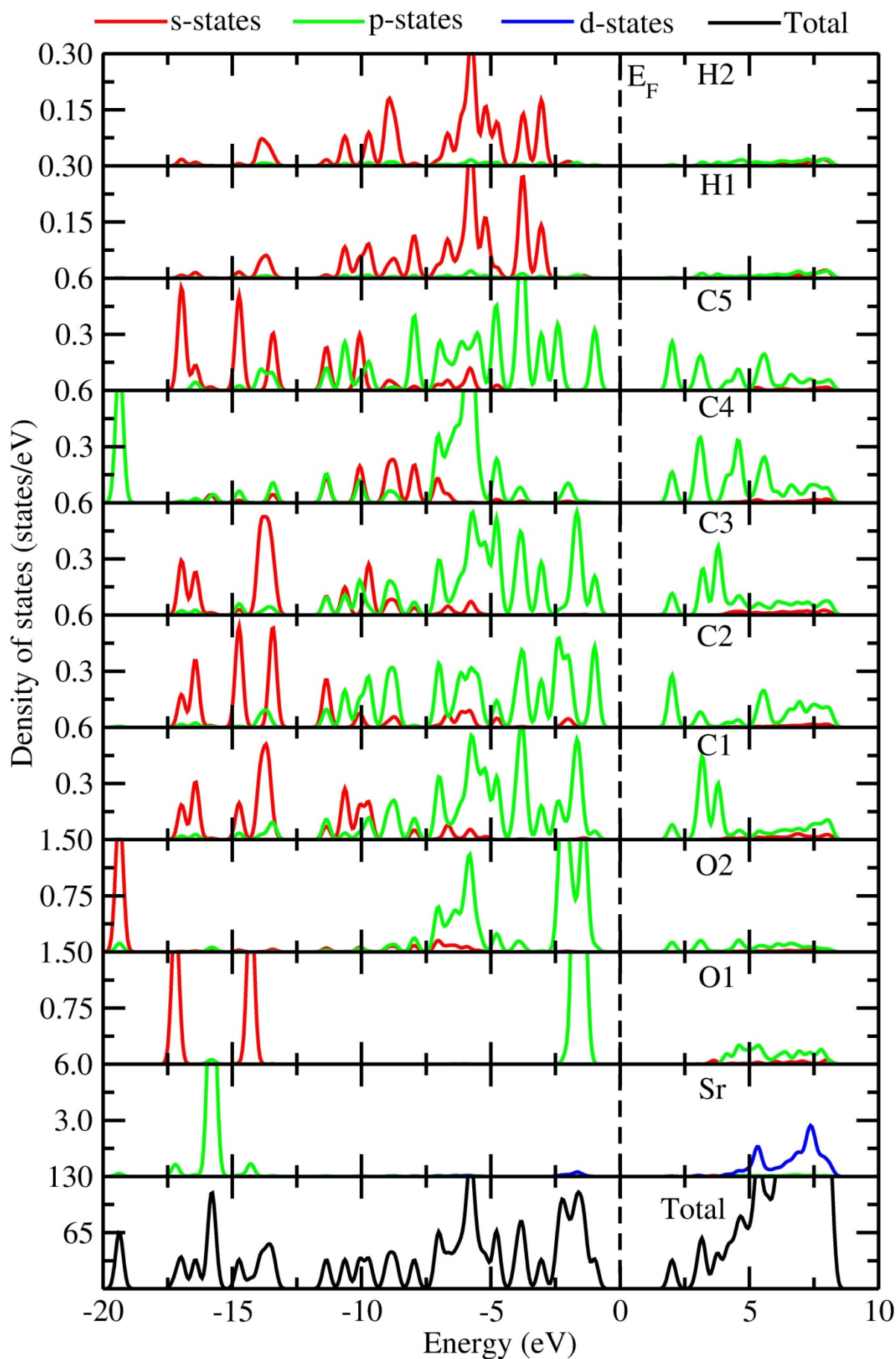


**Figure S9.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Mg-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

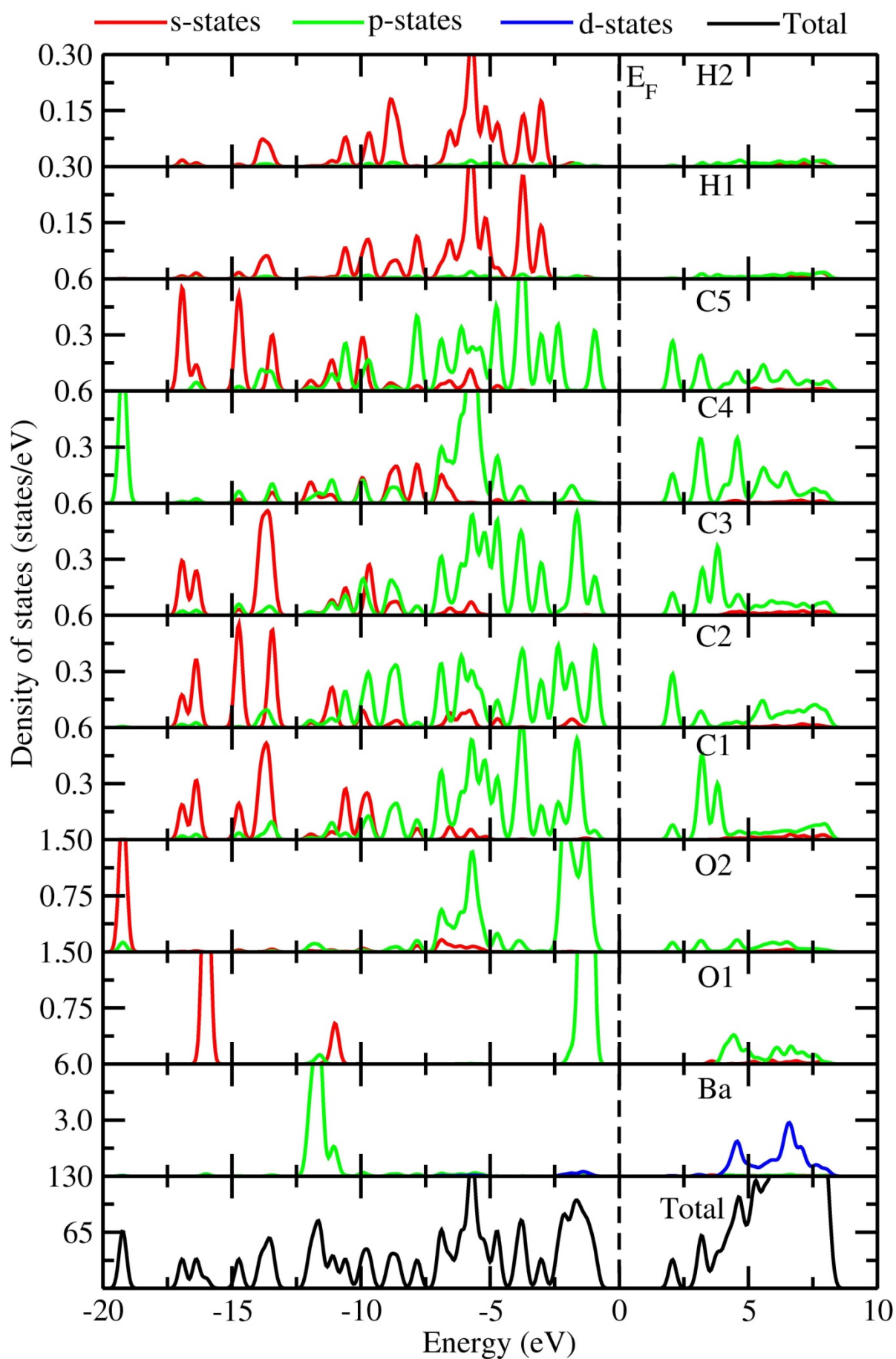




**Figure S10.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Ca-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

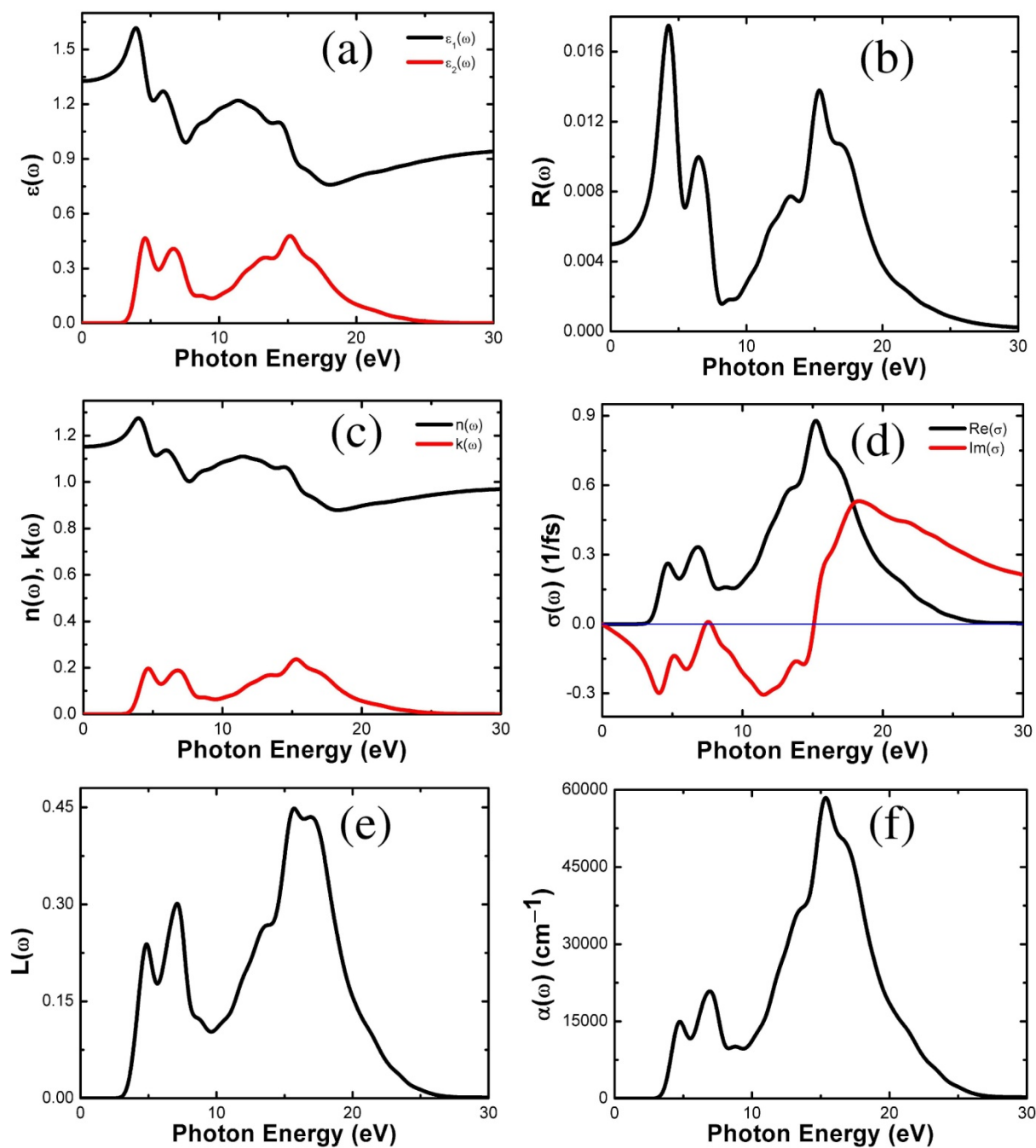


**Figure S11.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Sr-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

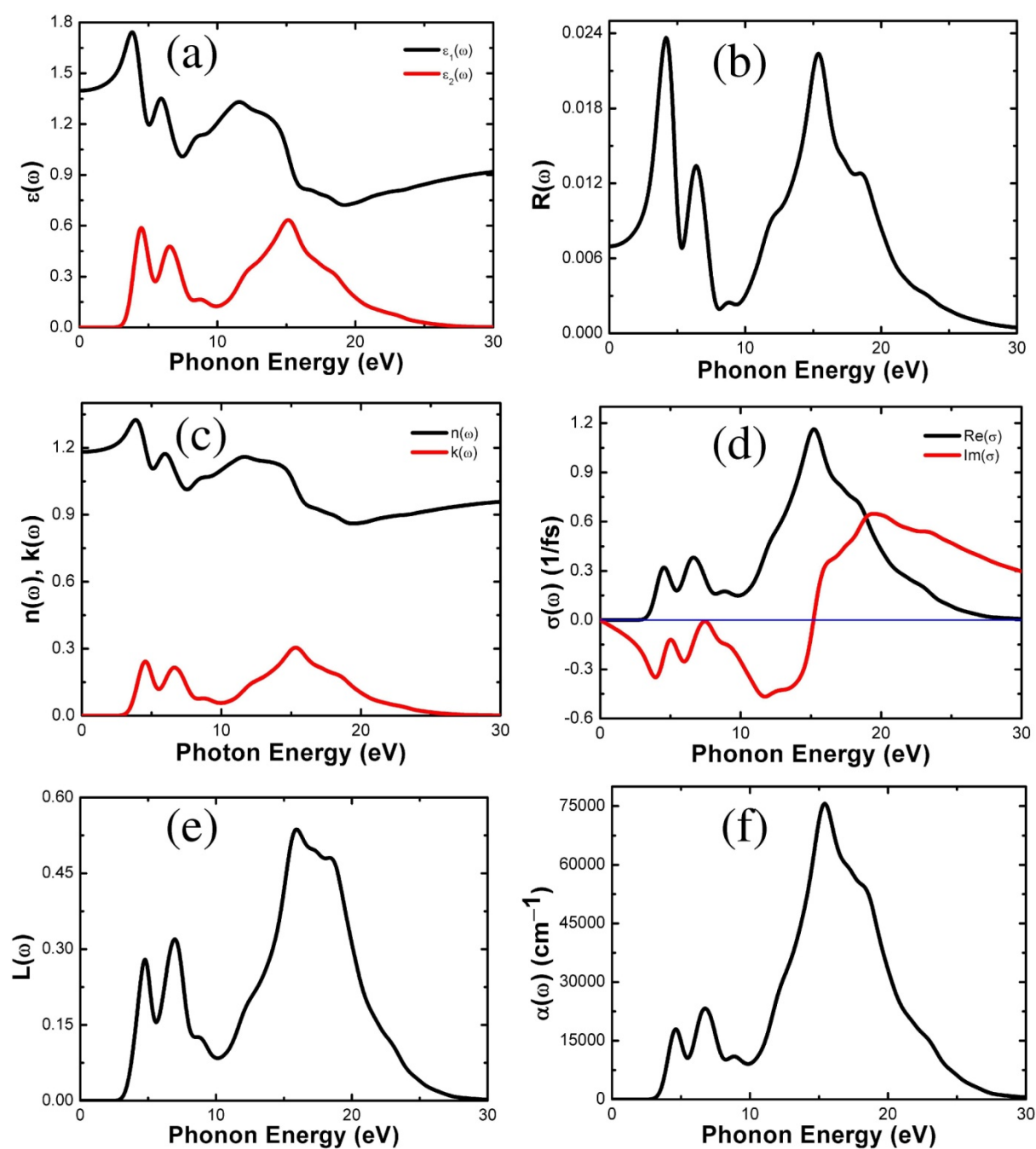


**Figure S12.** The calculated total density of states (TDOS) and partial density of states (PDOS) for Ba-IRMOF-10 in the cubic  $Fm-3m$  symmetry (no. 225)

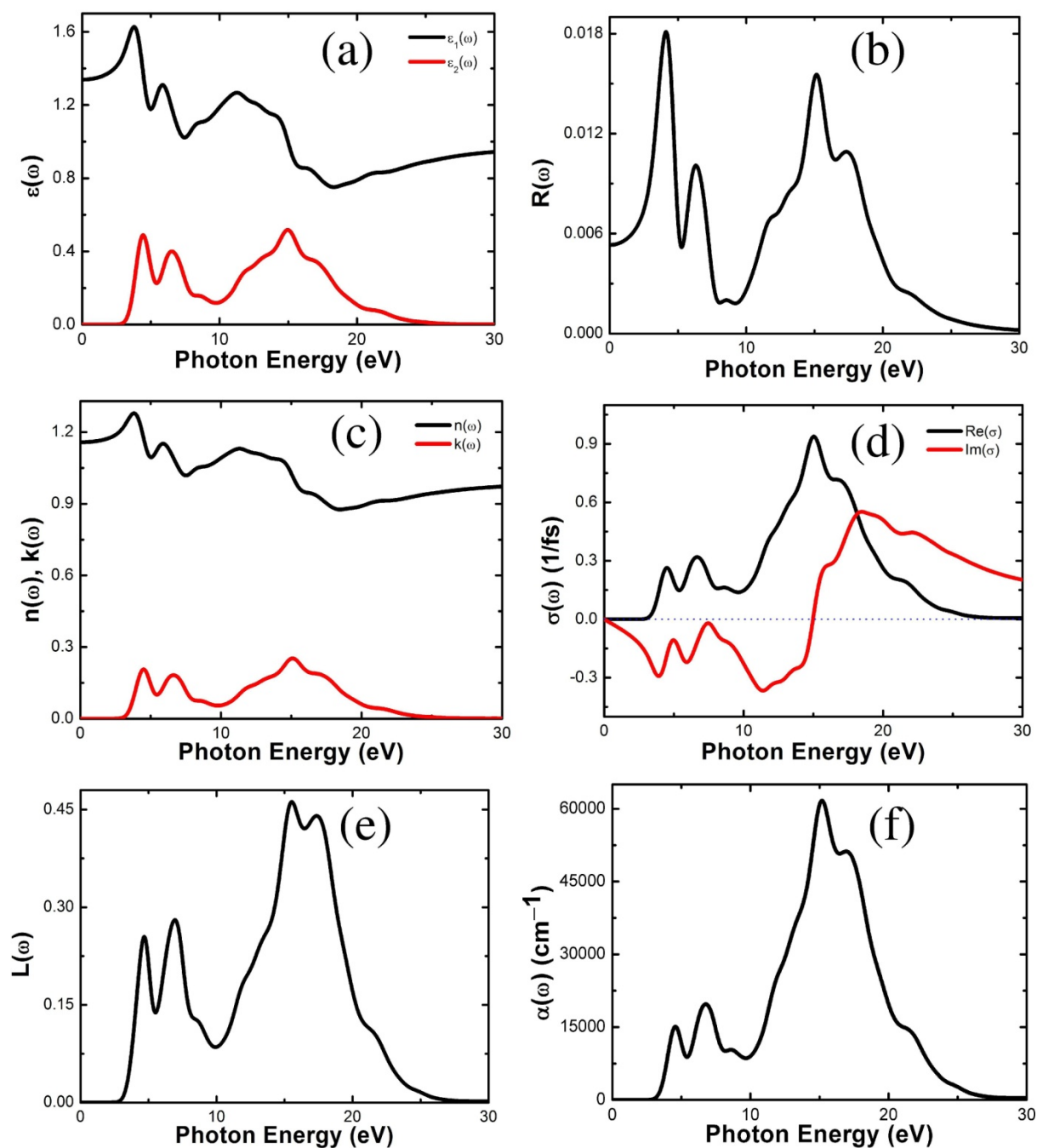




**Figure S13.** Calculated optical properties for Cd-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .

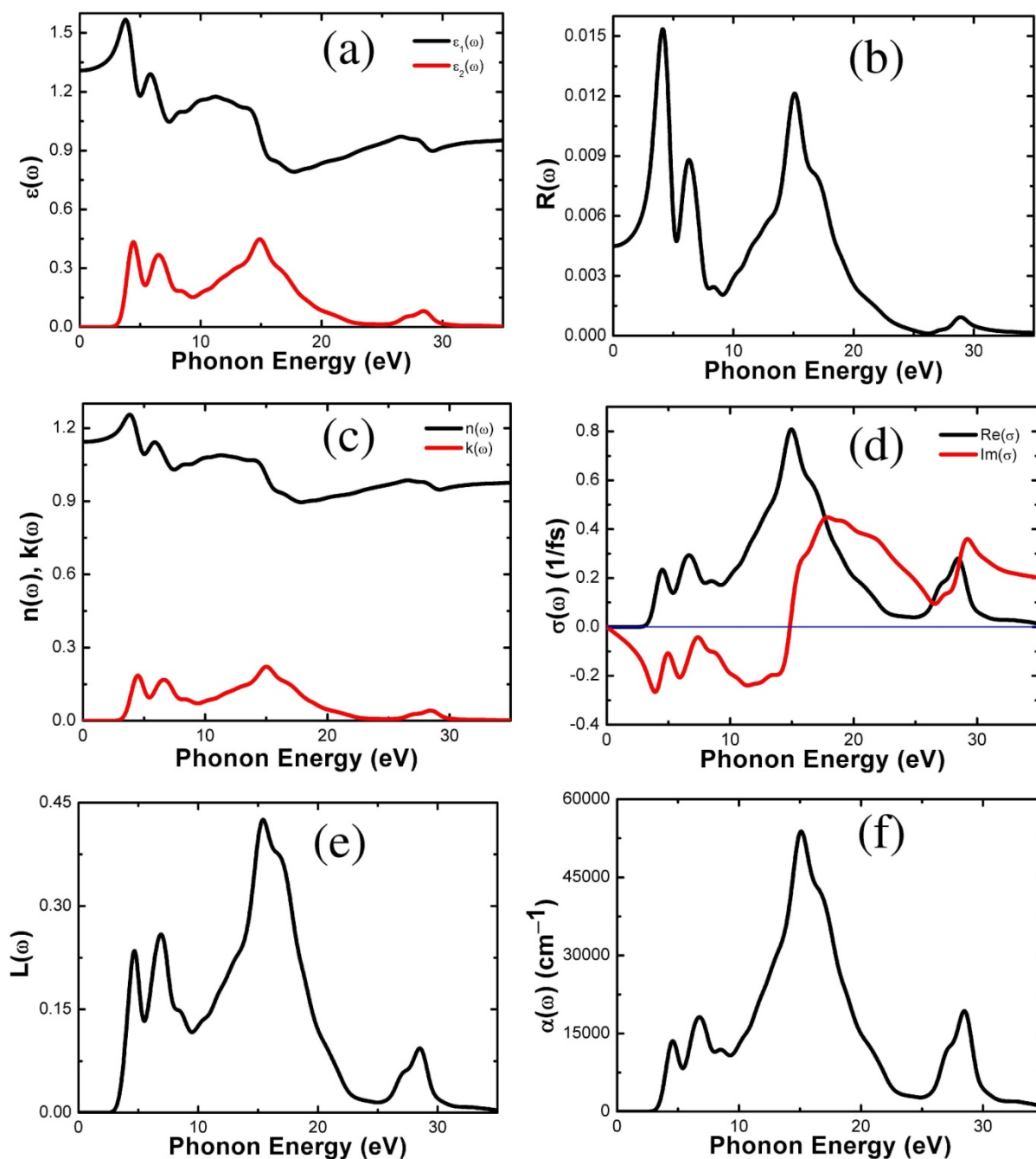


**Figure S14.** Calculated optical properties for Be-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .

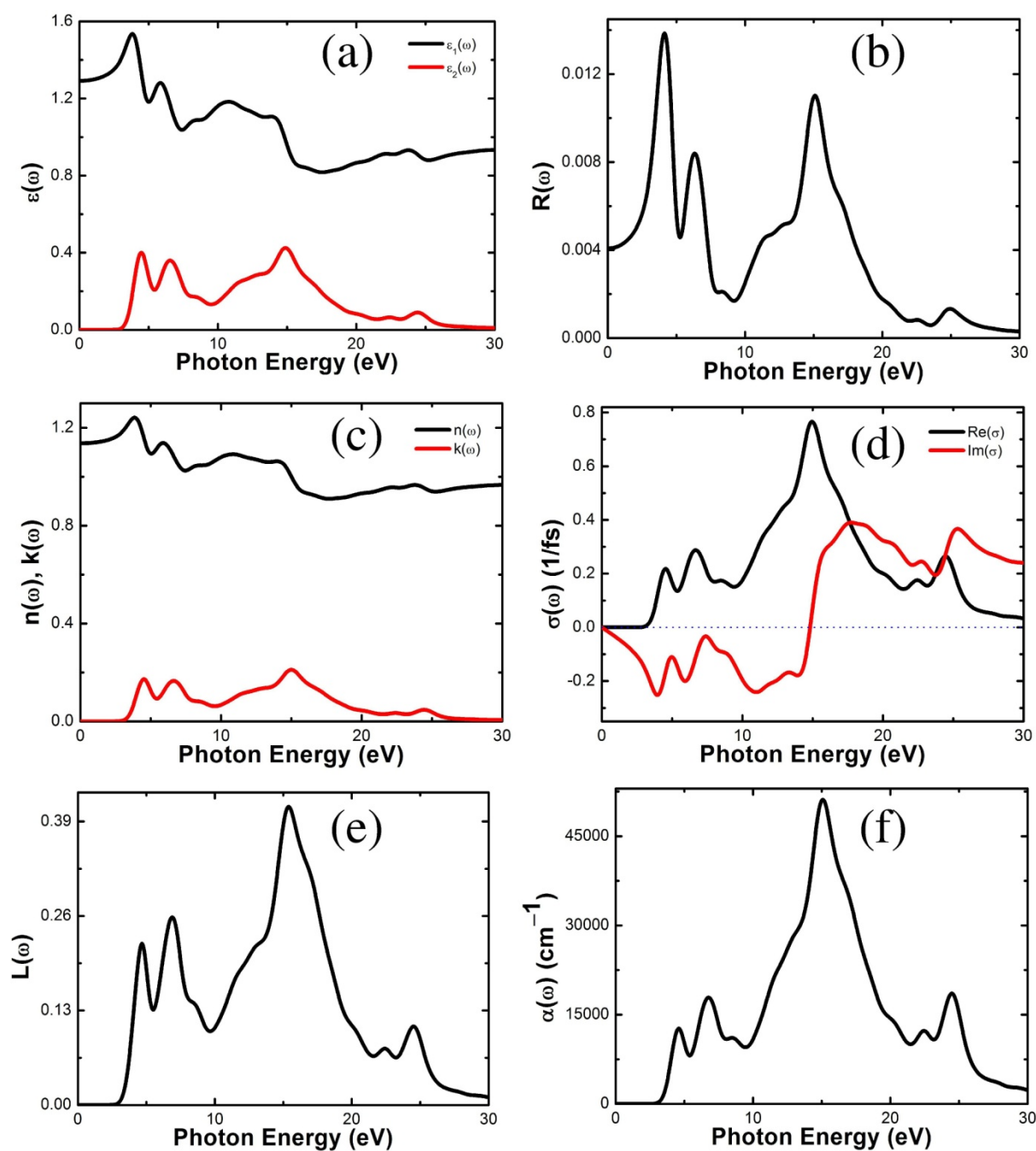


**Figure S15.** Calculated optical properties for Mg-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .

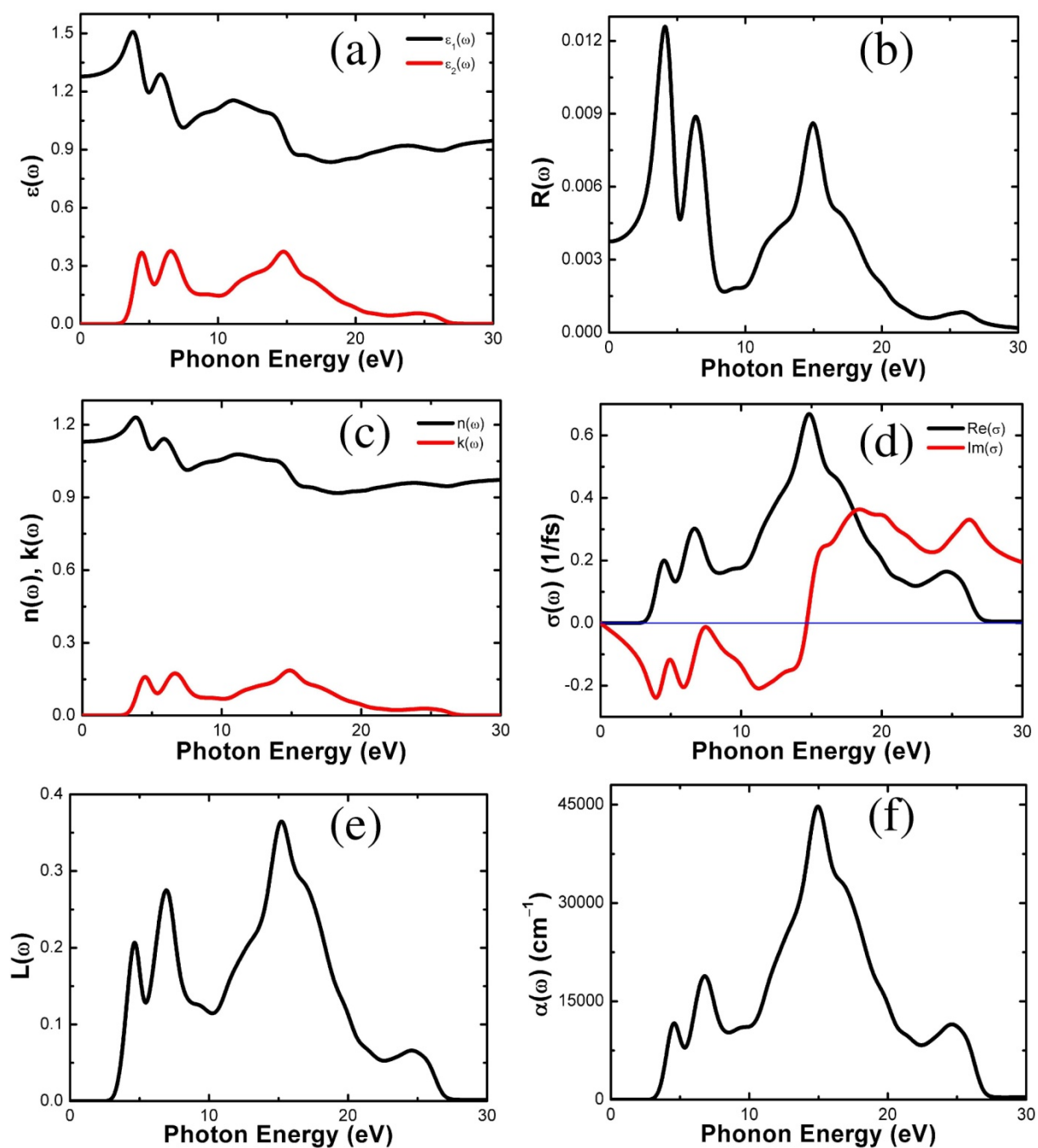




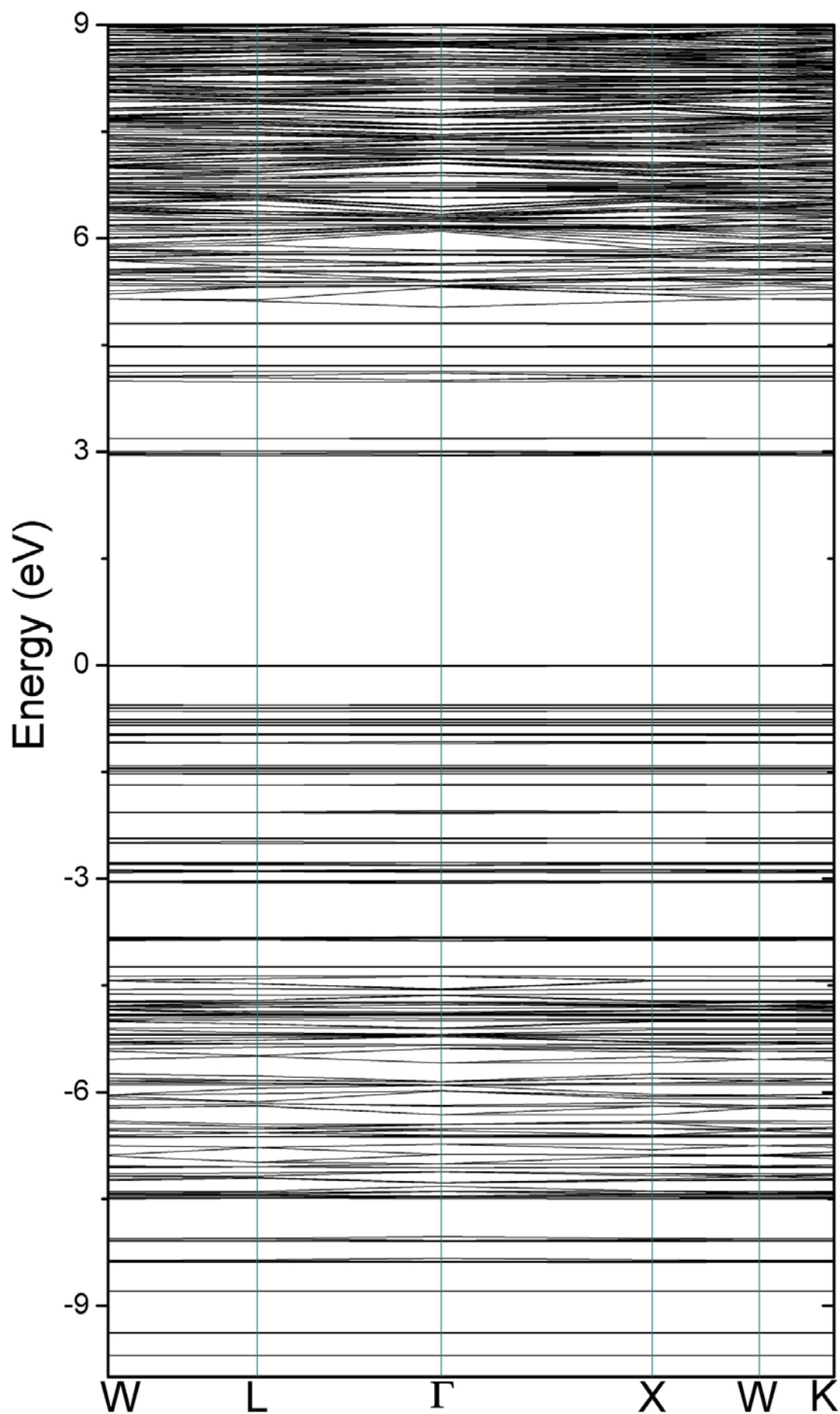
**Figure S16.** Calculated optical properties for Ca-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .



**Figure S17.** Calculated optical properties for Sr-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .

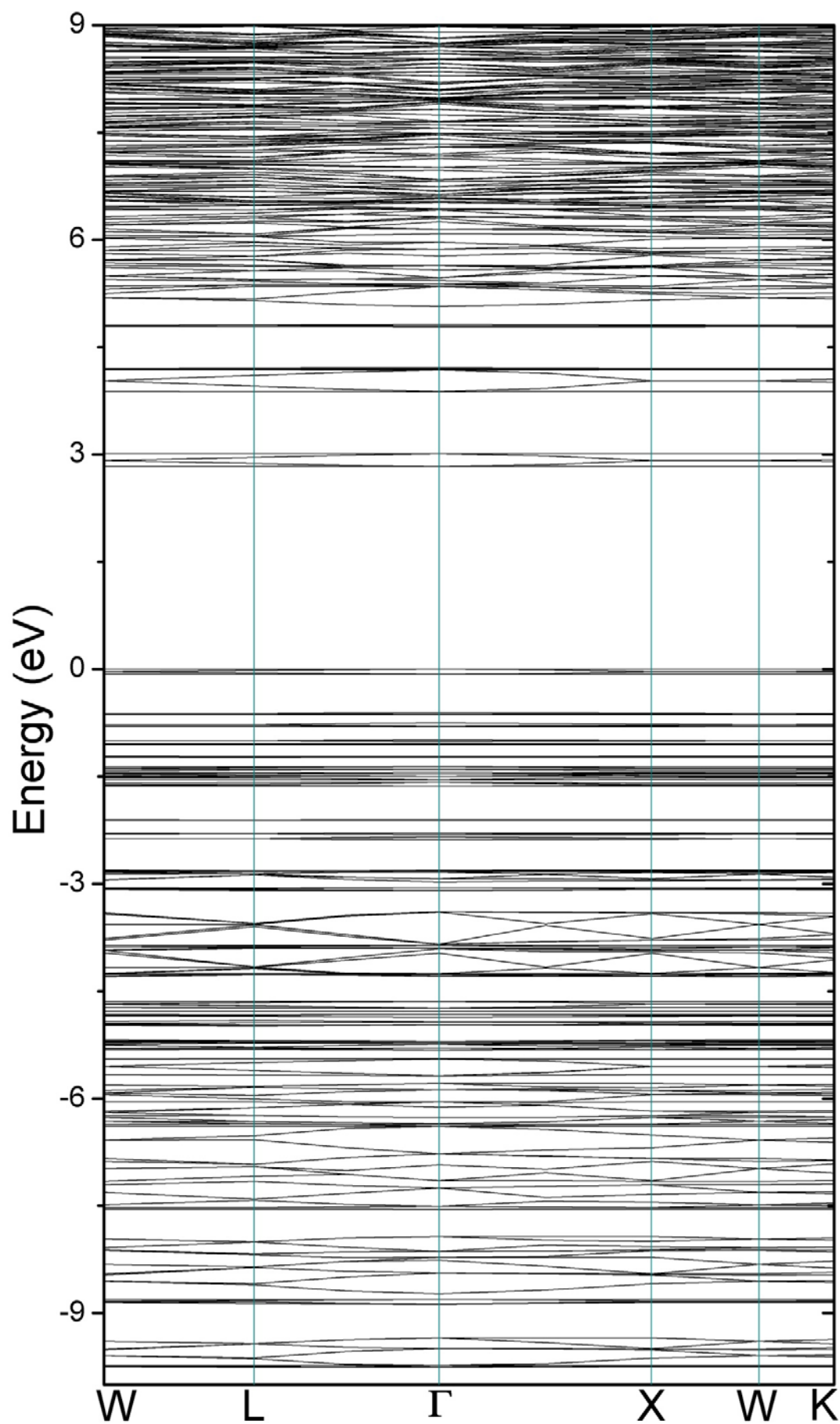


**Figure S18.** Calculated optical properties for Ba-IRMOF-10: (a) dielectric function  $\epsilon(\omega)$ , (b) reflectivity  $R(\omega)$ , (c) refractive index  $n(\omega)$ ; extinction coefficient  $k(\omega)$ , (d) optical conductivity  $\sigma(\omega)$ , (e) energy loss function  $L(\omega)$ , (f) absorption  $\alpha(\omega)$ .

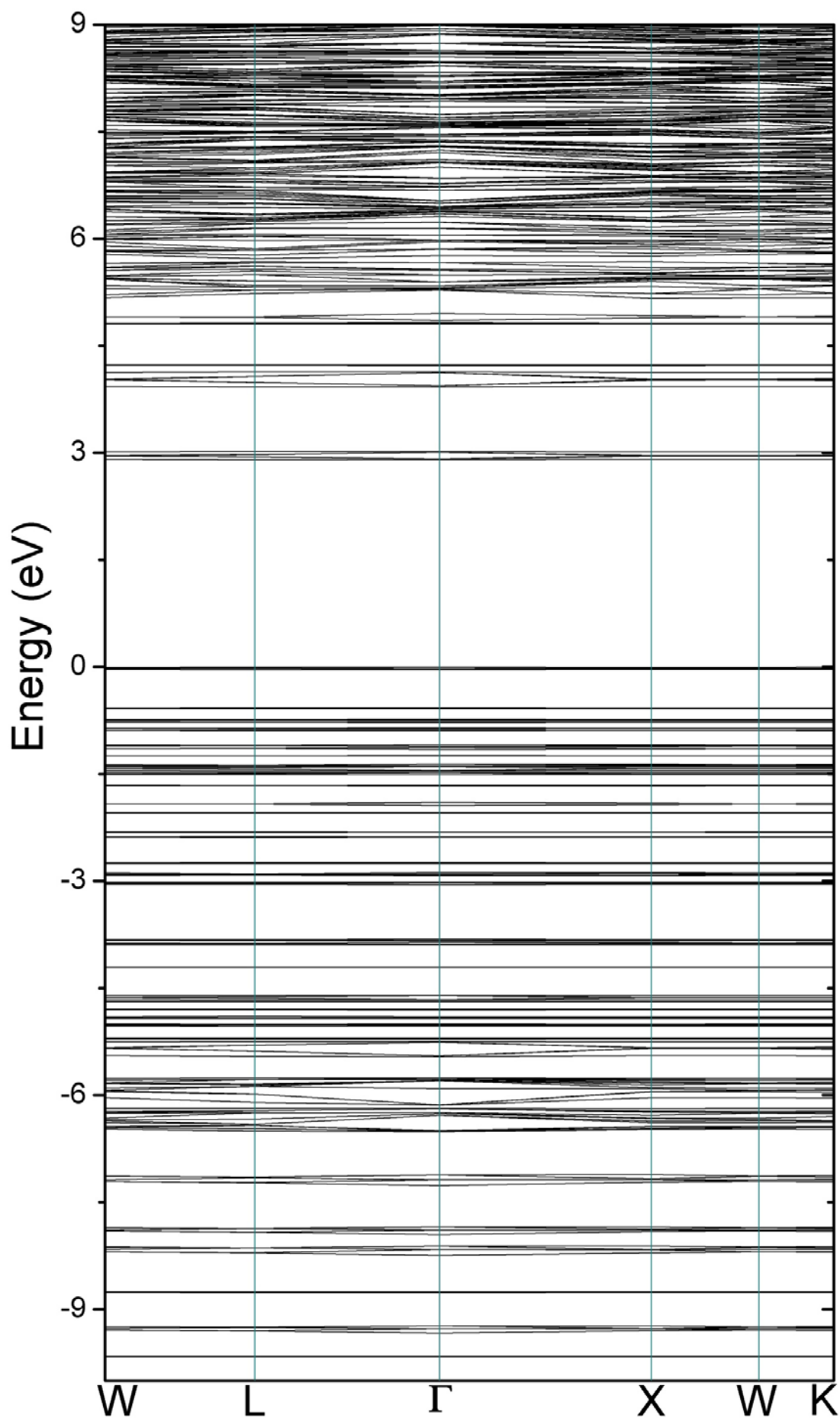


**Figure S19.** The electronic band structure of Cd-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

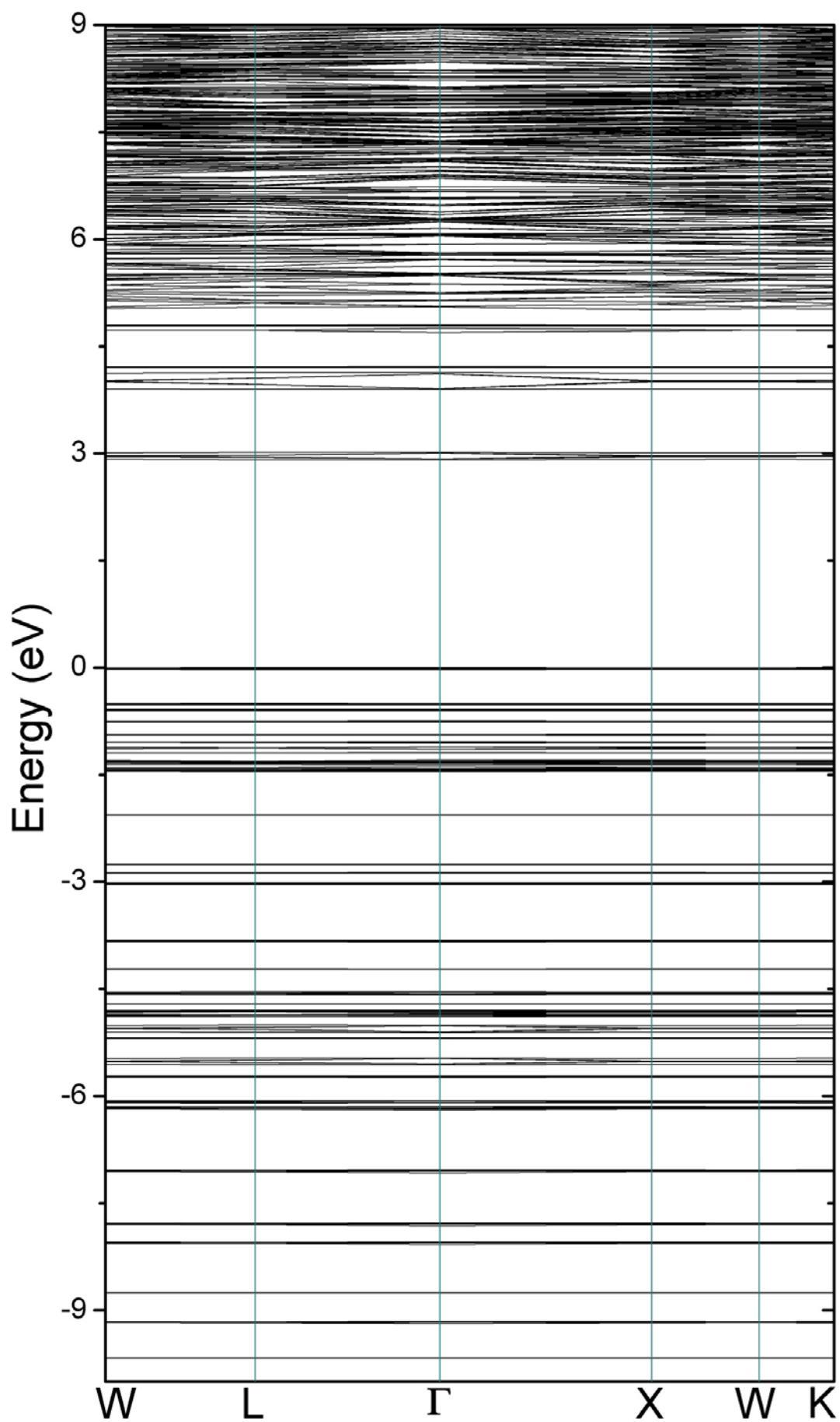




**Figure S20.** The electronic band structure of Be-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

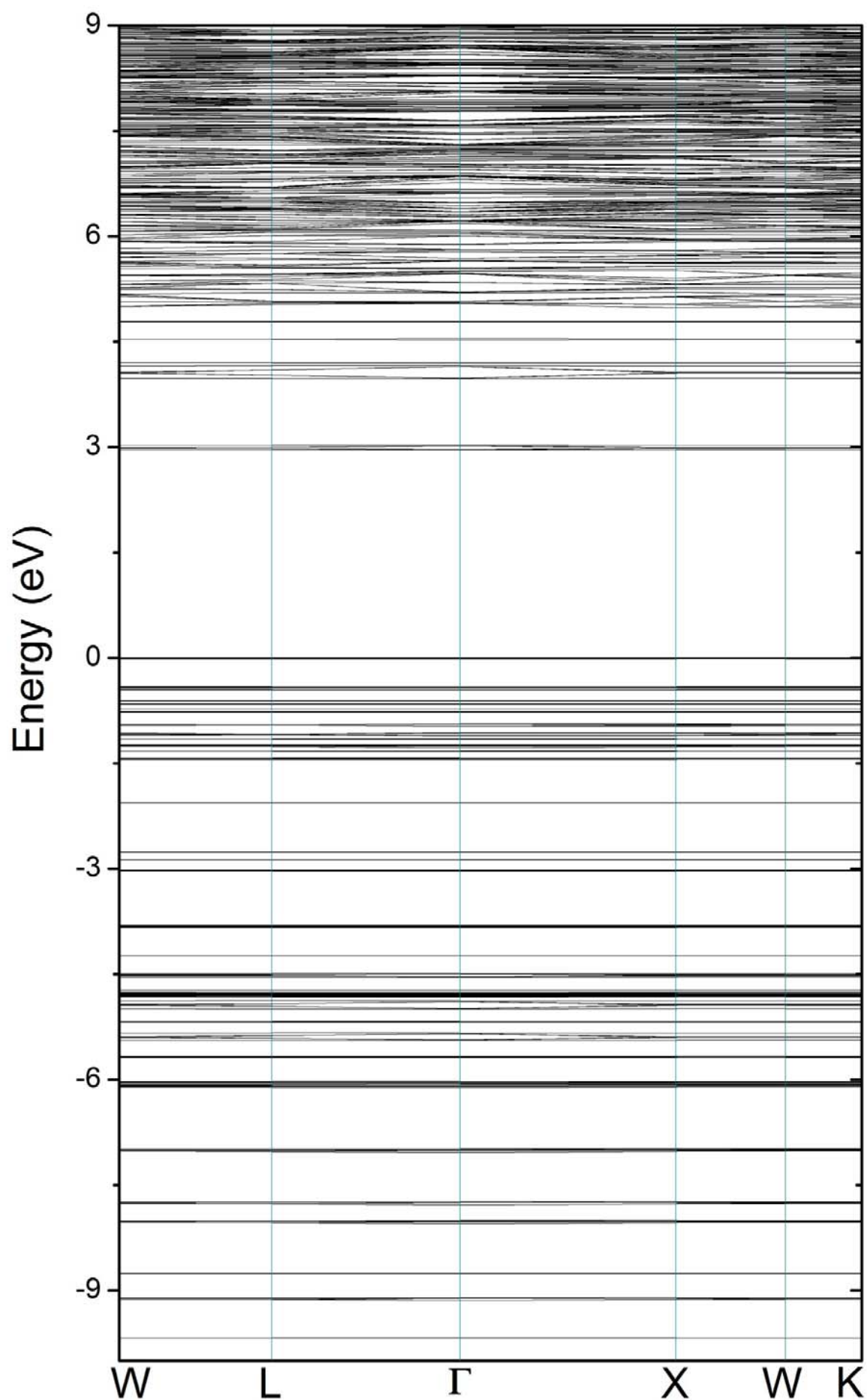


**Figure S21.** The electronic band structure of Mg-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

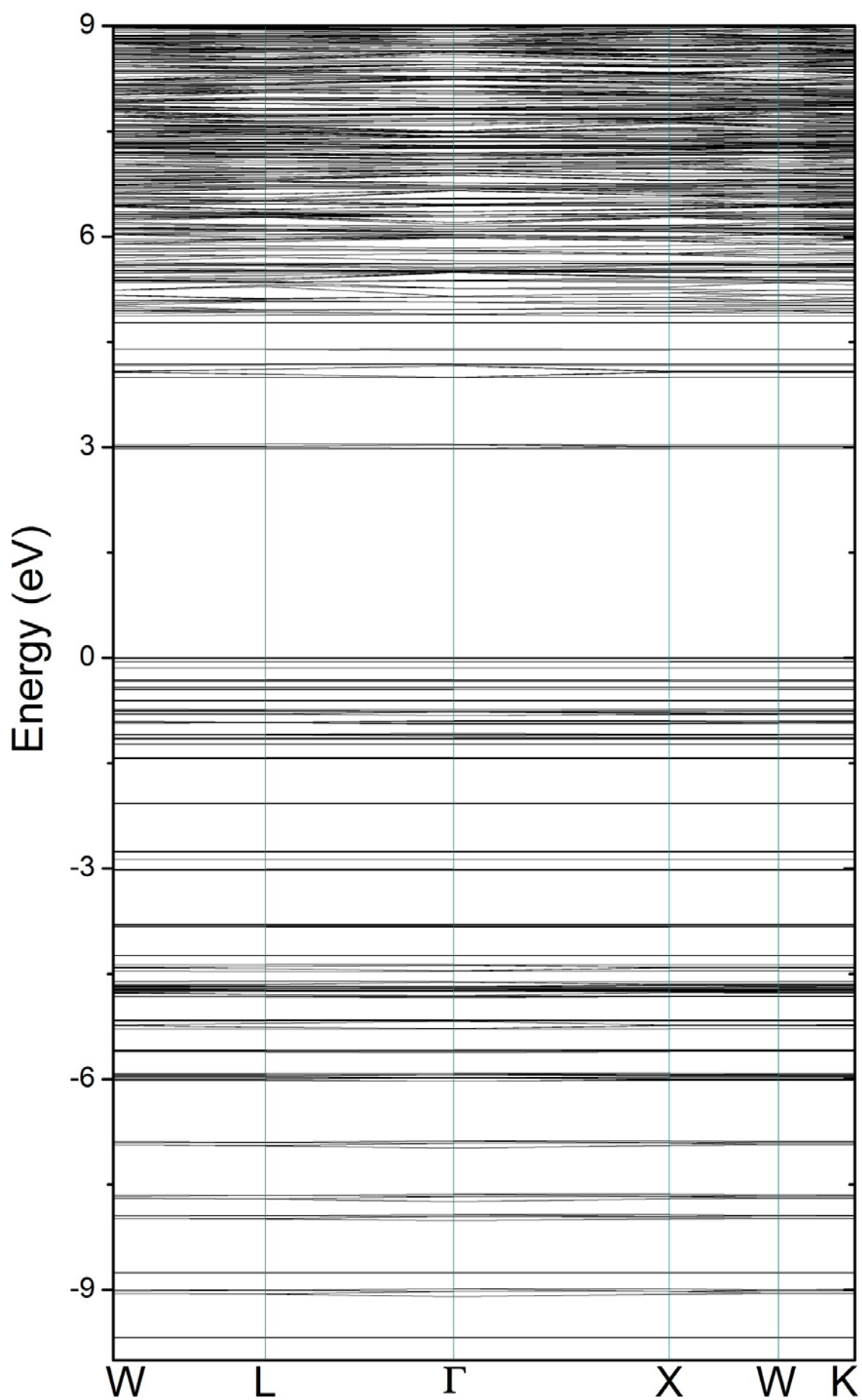


**Figure S22.** The electronic band structure of Ca-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.





**Figure S23.** The electronic band structure of Sr-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.



**Figure S24.** The electronic band structure of Ba-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.