Electronic Supplementary Material (ESI) for RSC Advances

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

Supporting Information

Li-Ming Yang*[†], Ponniah Ravindran[‡], Ponniah Vajeeston[‡], and Mats Tilset*[†]

[†]*Center of Theoretical and Computational Chemistry, Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, N-0315 Oslo, Norway,* [‡]*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 and l.m.yang@kjemi.uio.no.; Fax: +47 22855441;)

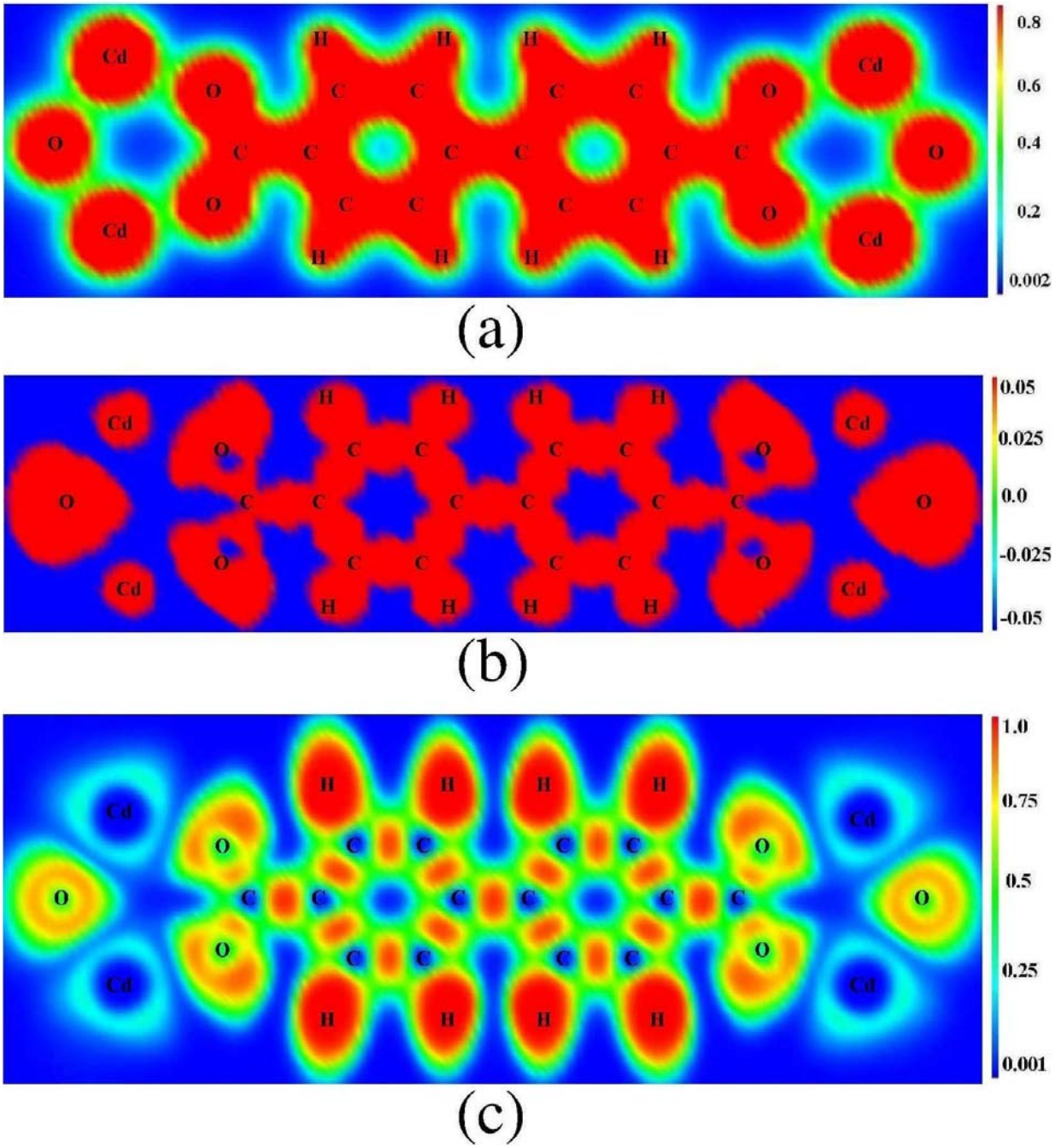

Figure S1. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Cd-IRMOF-10 in the (110) plane.

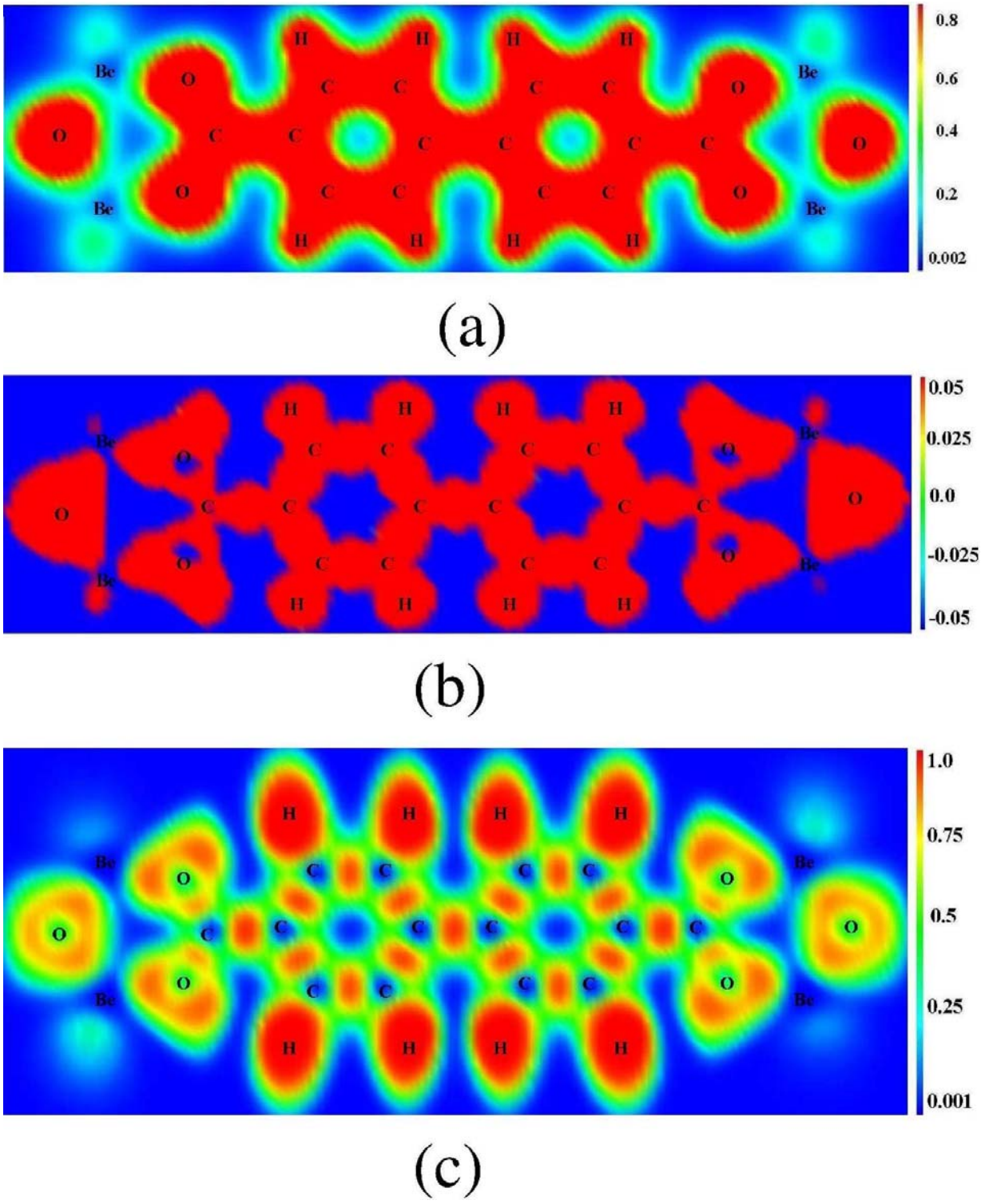

Figure S2. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Be-IRMOF-10 in the (110) plane.

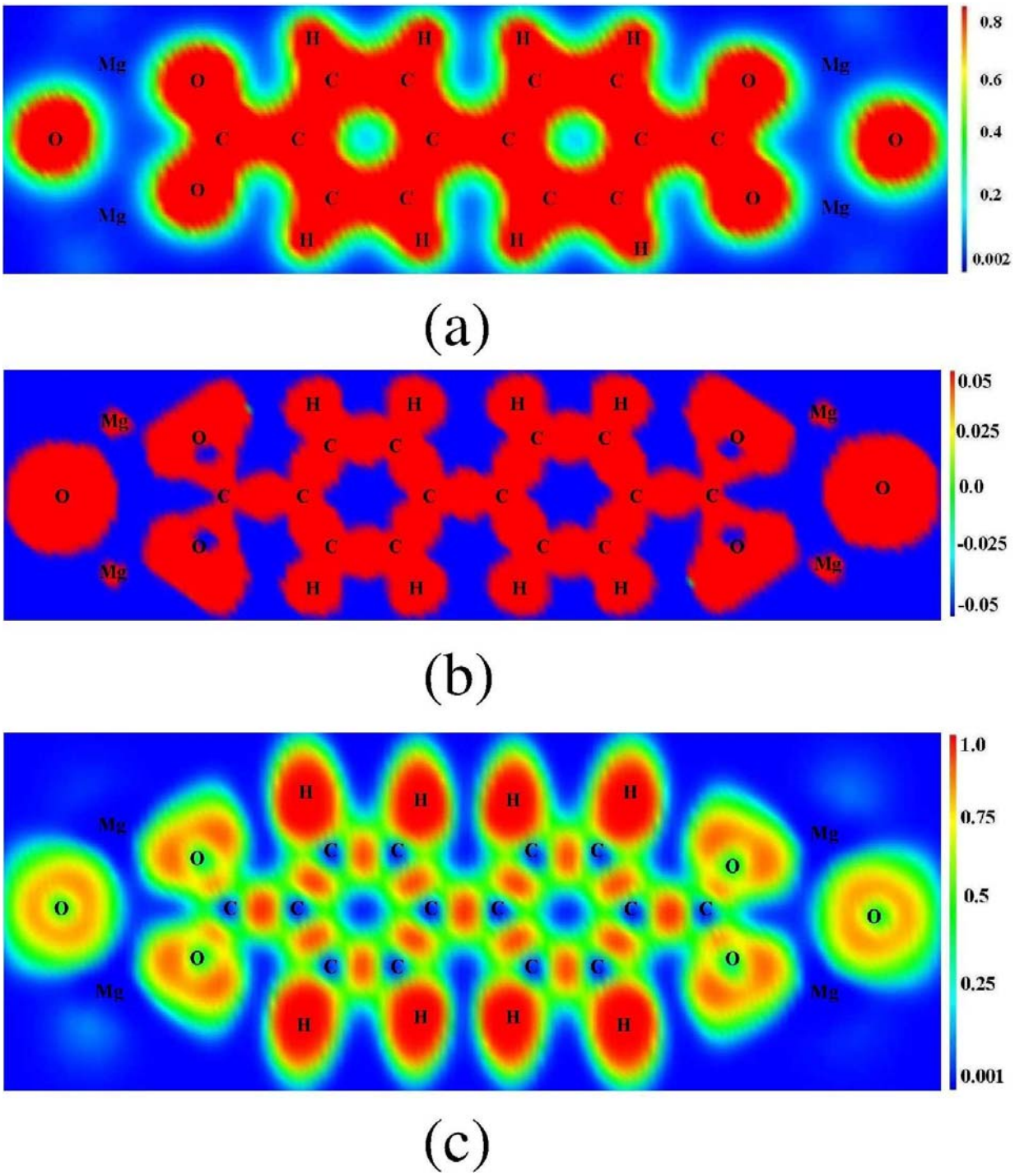

Figure S3. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Mg-IRMOF-10 in the (110) plane.

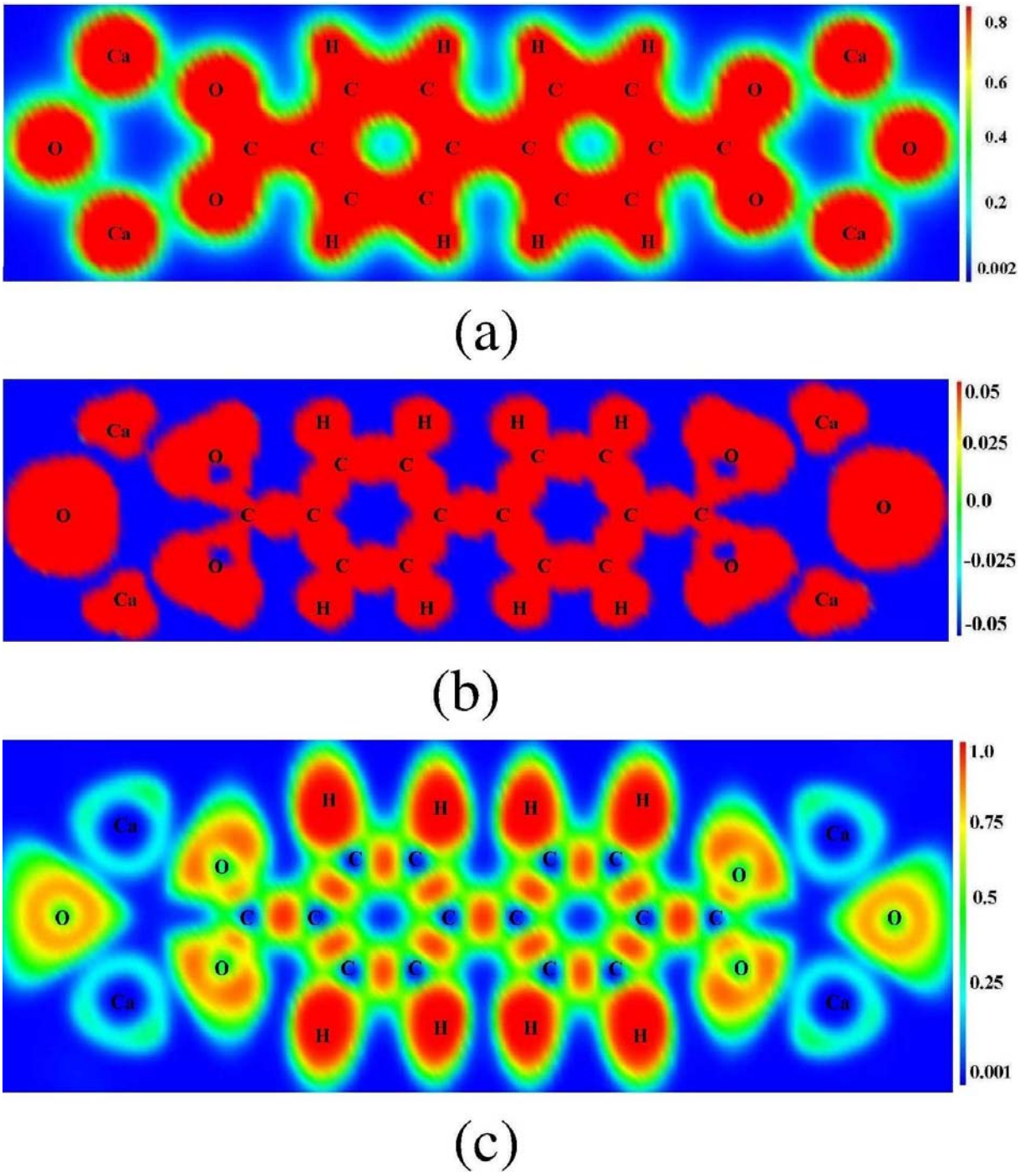

Figure S4. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Ca-IRMOF-10 in the (110) plane.

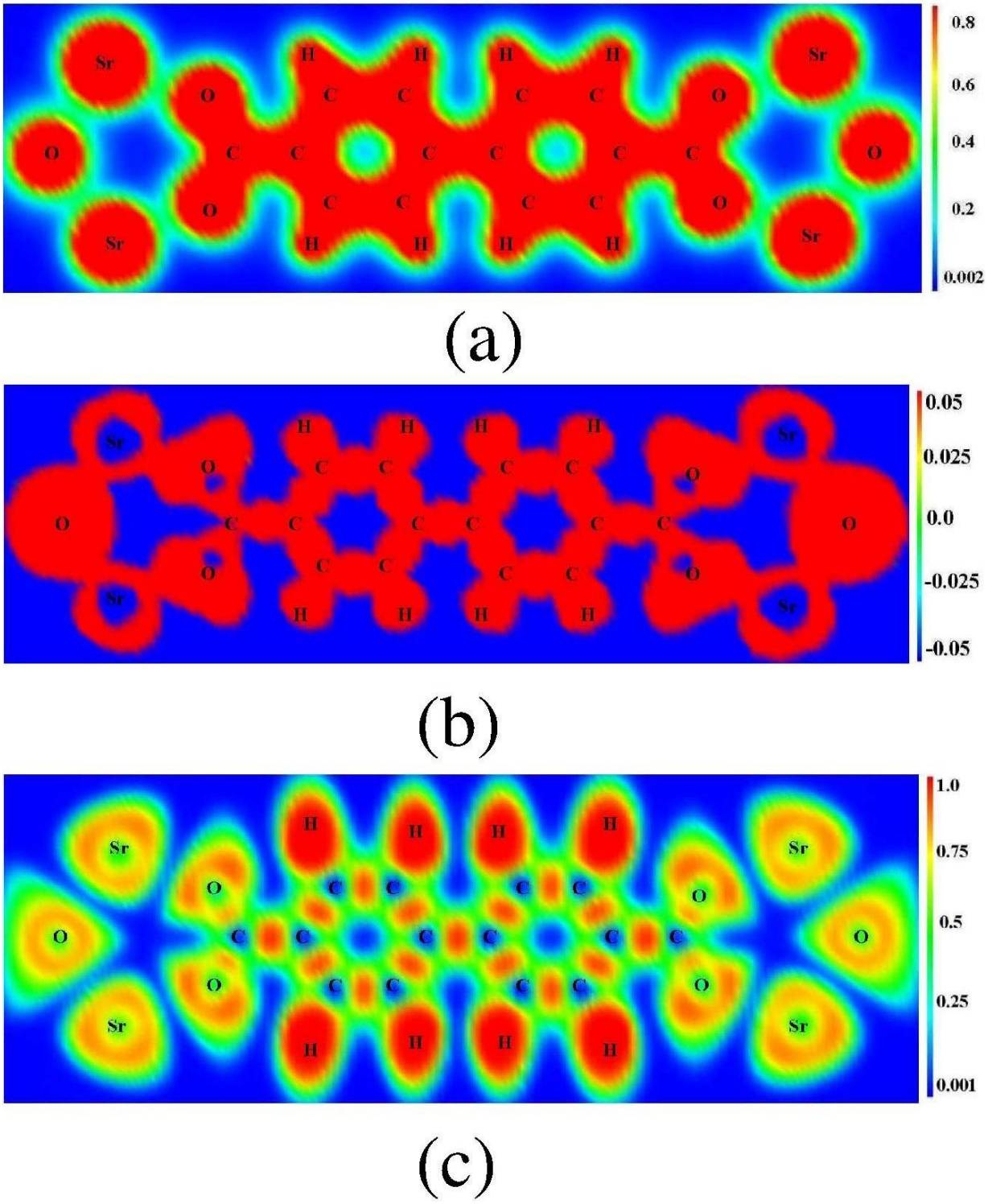

Figure S5. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Sr-IRMOF-10 in the (110) plane.

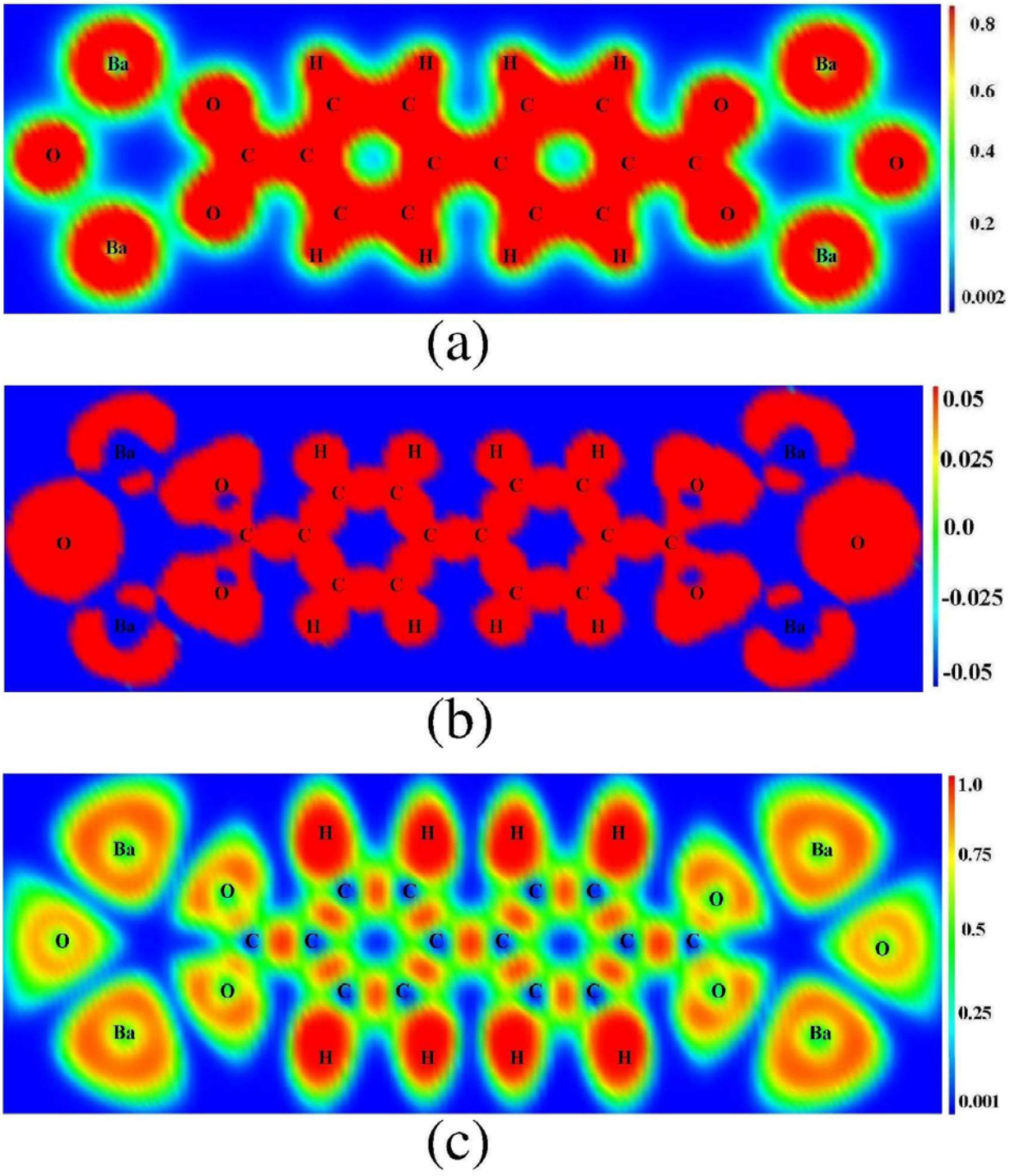

Figure S6. Calculated charge density (a), charge transfer (b), and electron localization function (c) plots for Ba-IRMOF-10 in the (110) plane.

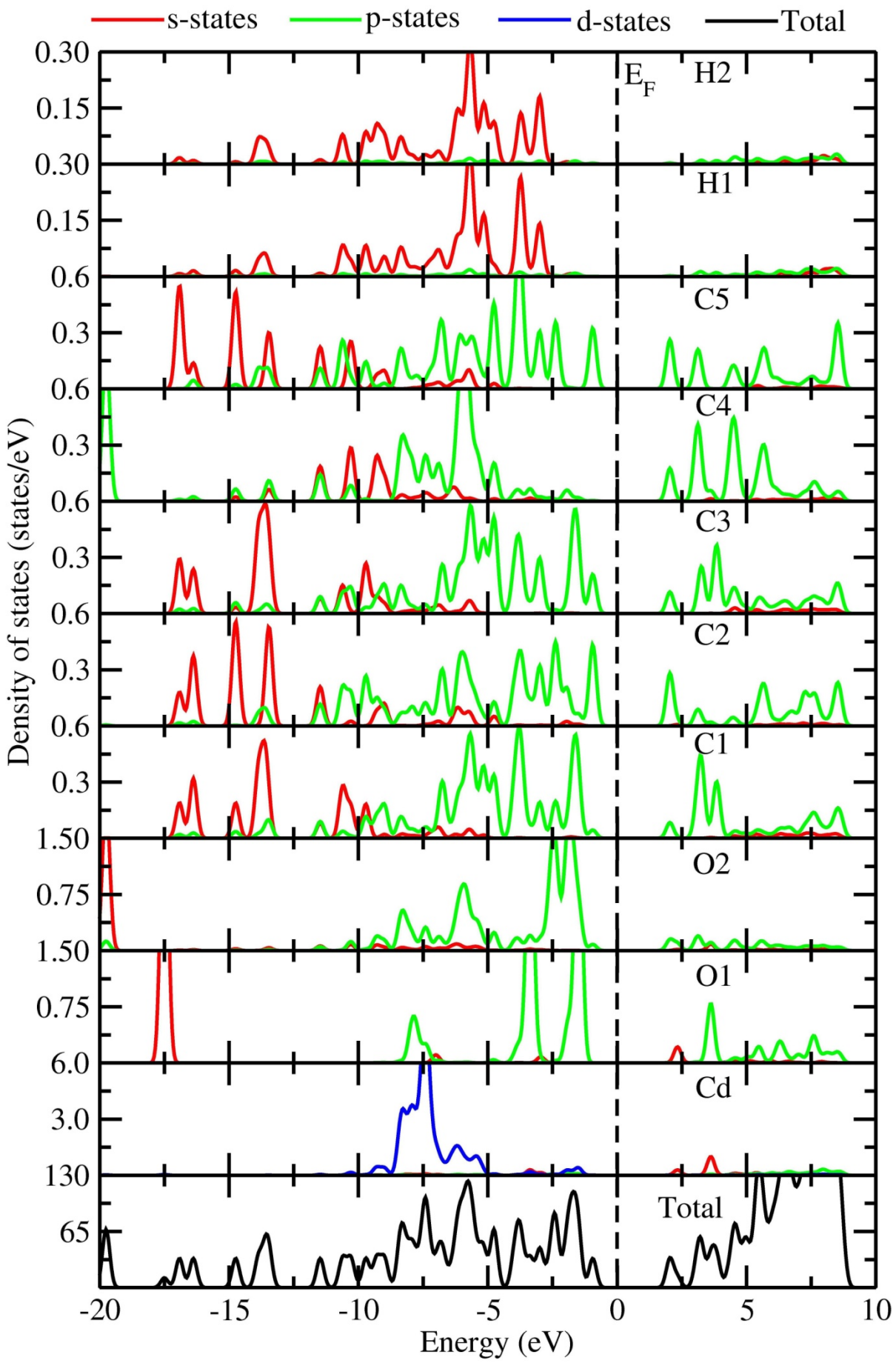

Figure S7. The calculated total density of states (TDOS) and partial density of states (PDOS) for Cd-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

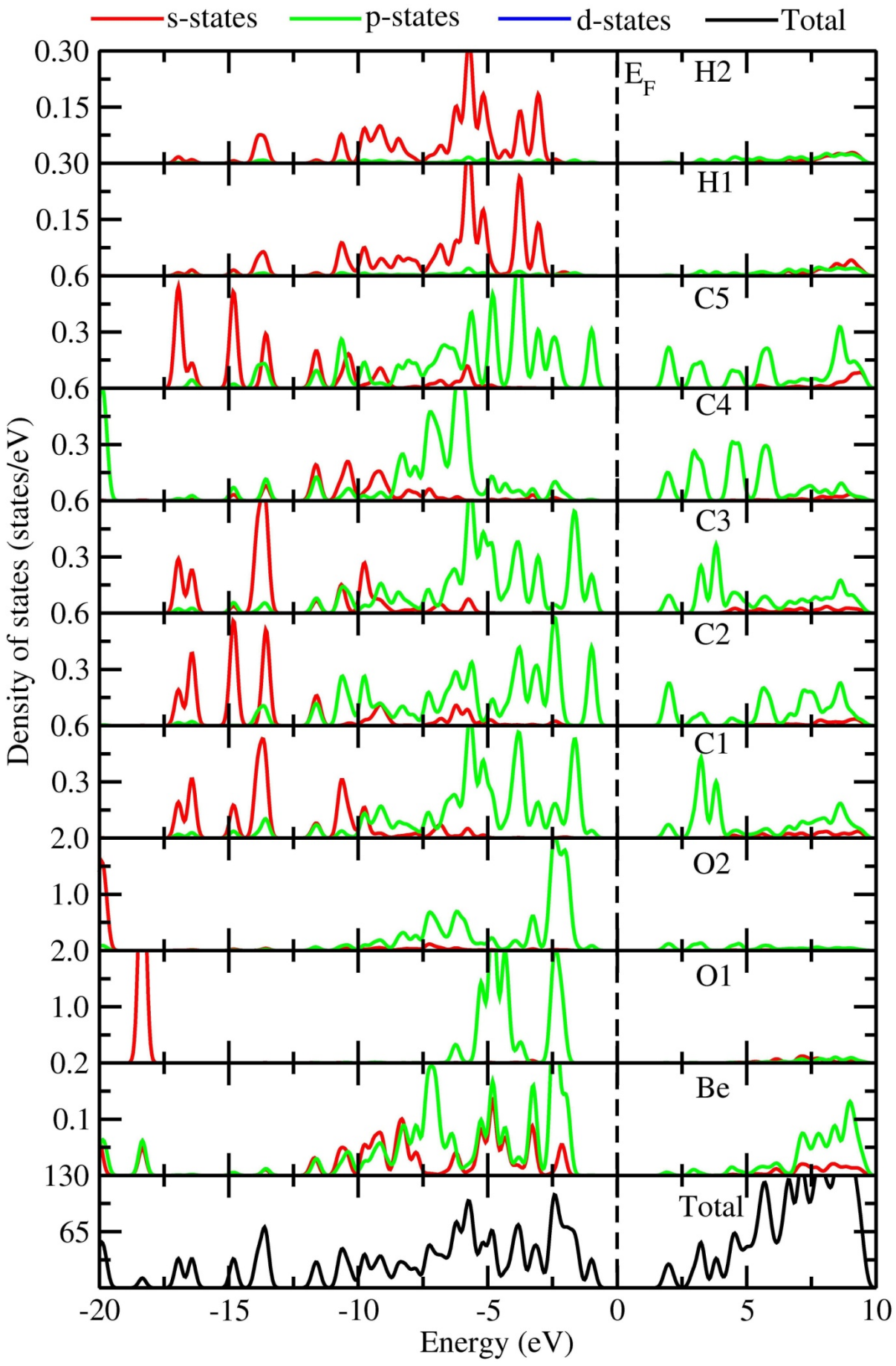

Figure S8. The calculated total density of states (TDOS) and partial density of states (PDOS) for Be-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

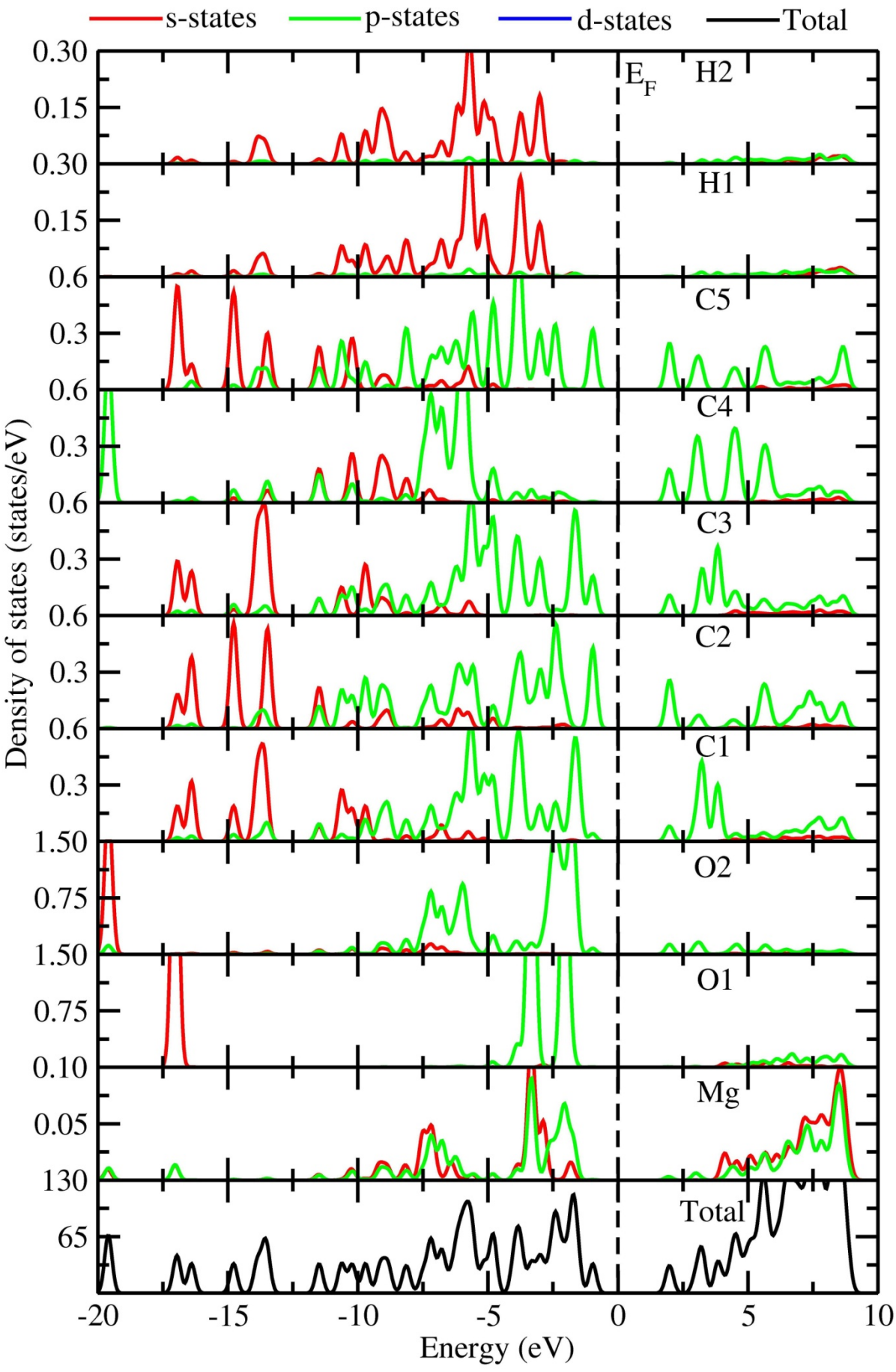

Figure S9. The calculated total density of states (TDOS) and partial density of states (PDOS) for Mg-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

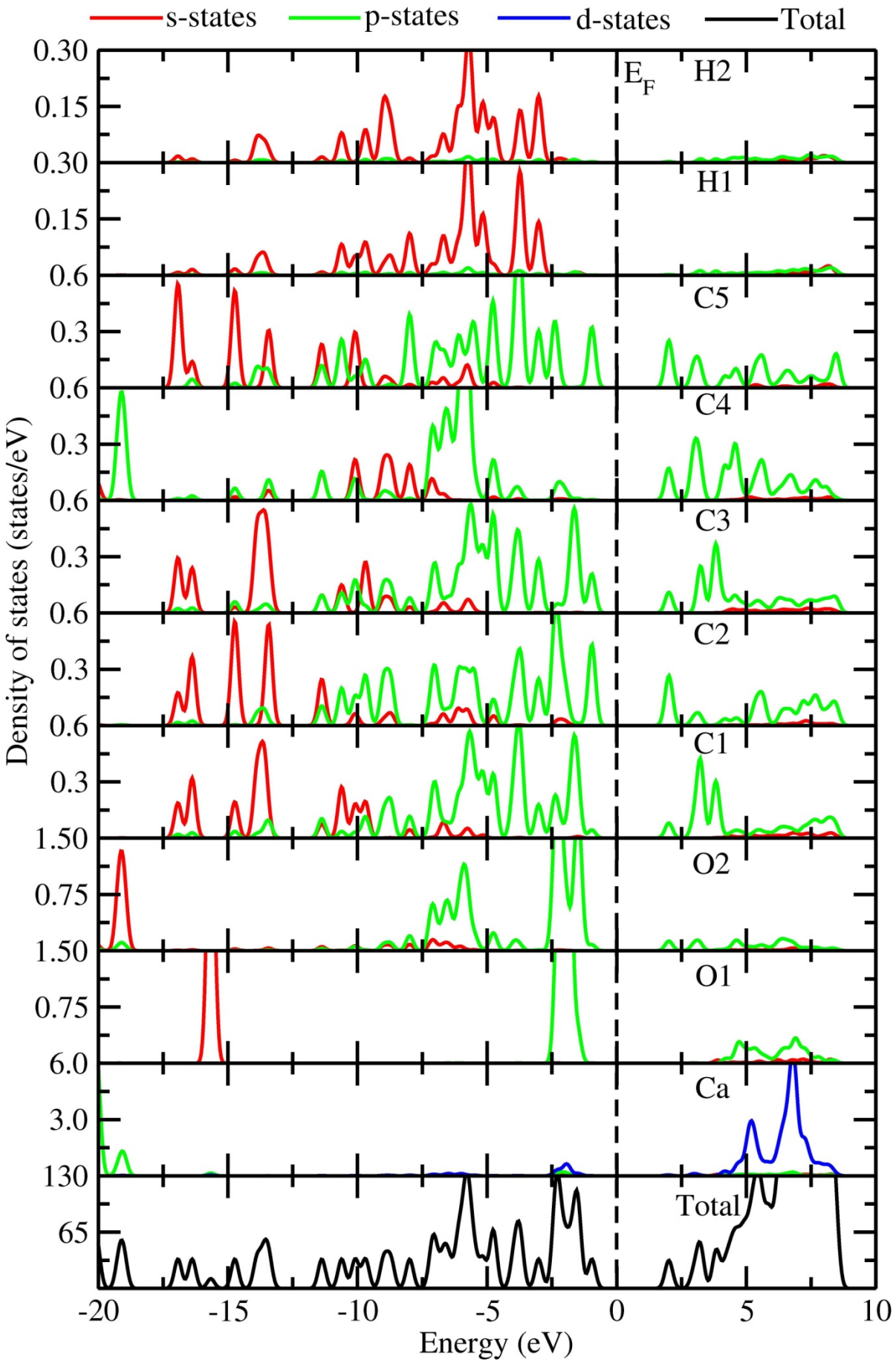

Figure S10. The calculated total density of states (TDOS) and partial density of states (PDOS) for Ca-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

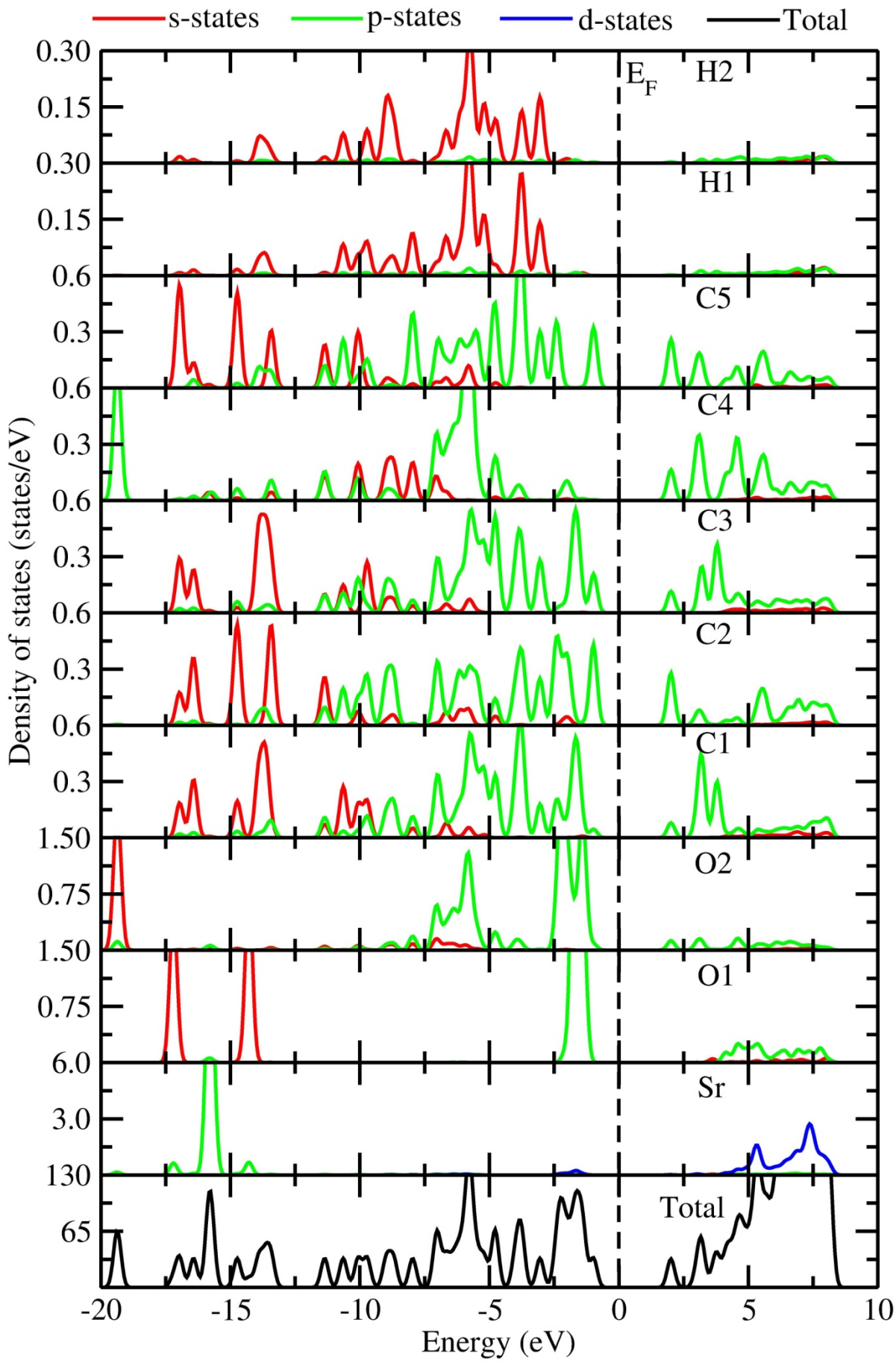

Figure S11. The calculated total density of states (TDOS) and partial density of states (PDOS) for Sr-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

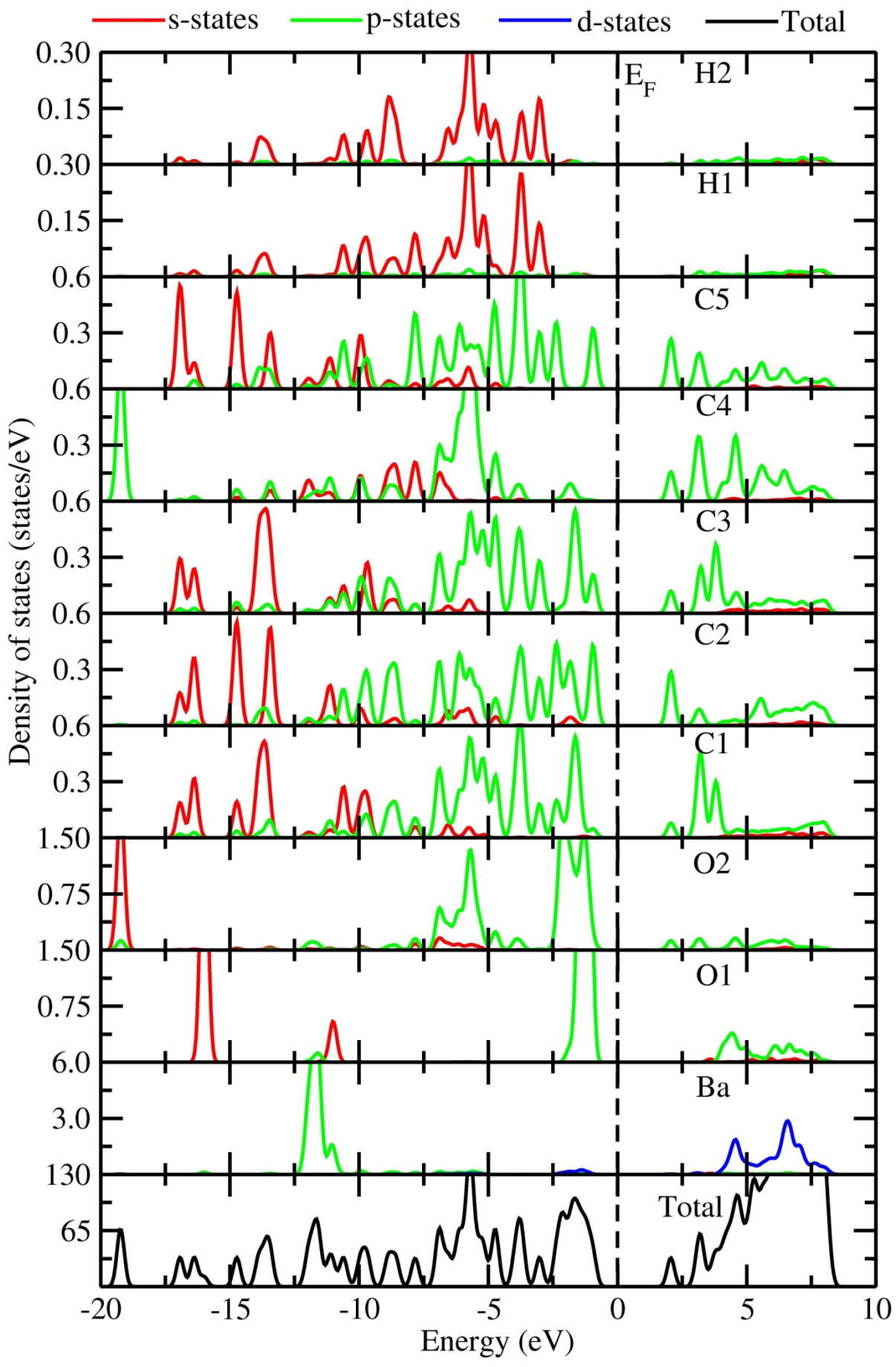

Figure S12. The calculated total density of states (TDOS) and partial density of states (PDOS) for Ba-IRMOF-10 in the cubic *Fm-3m* symmetry (no. 225)

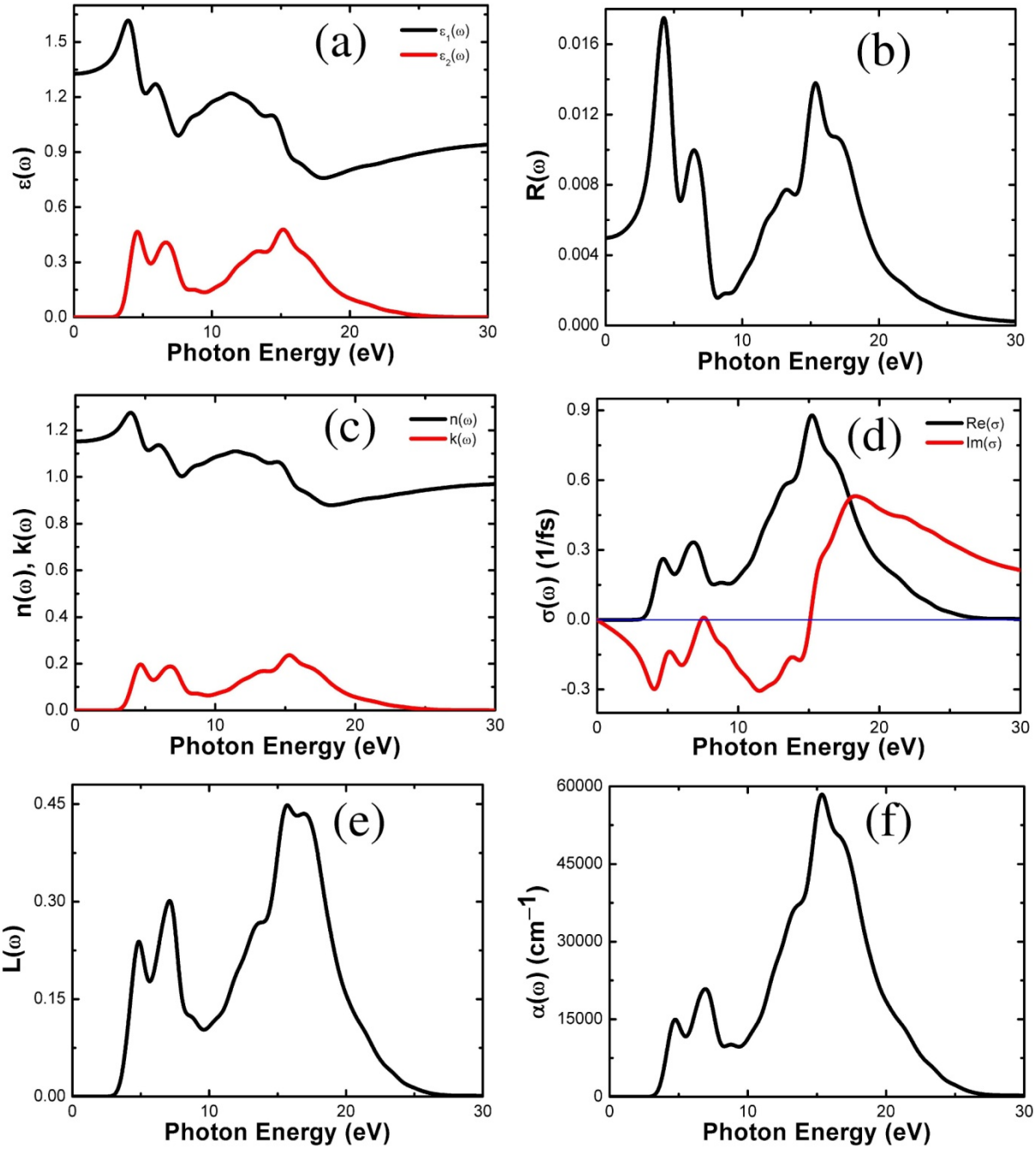

Figure S13. Calculated optical properties for Cd-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

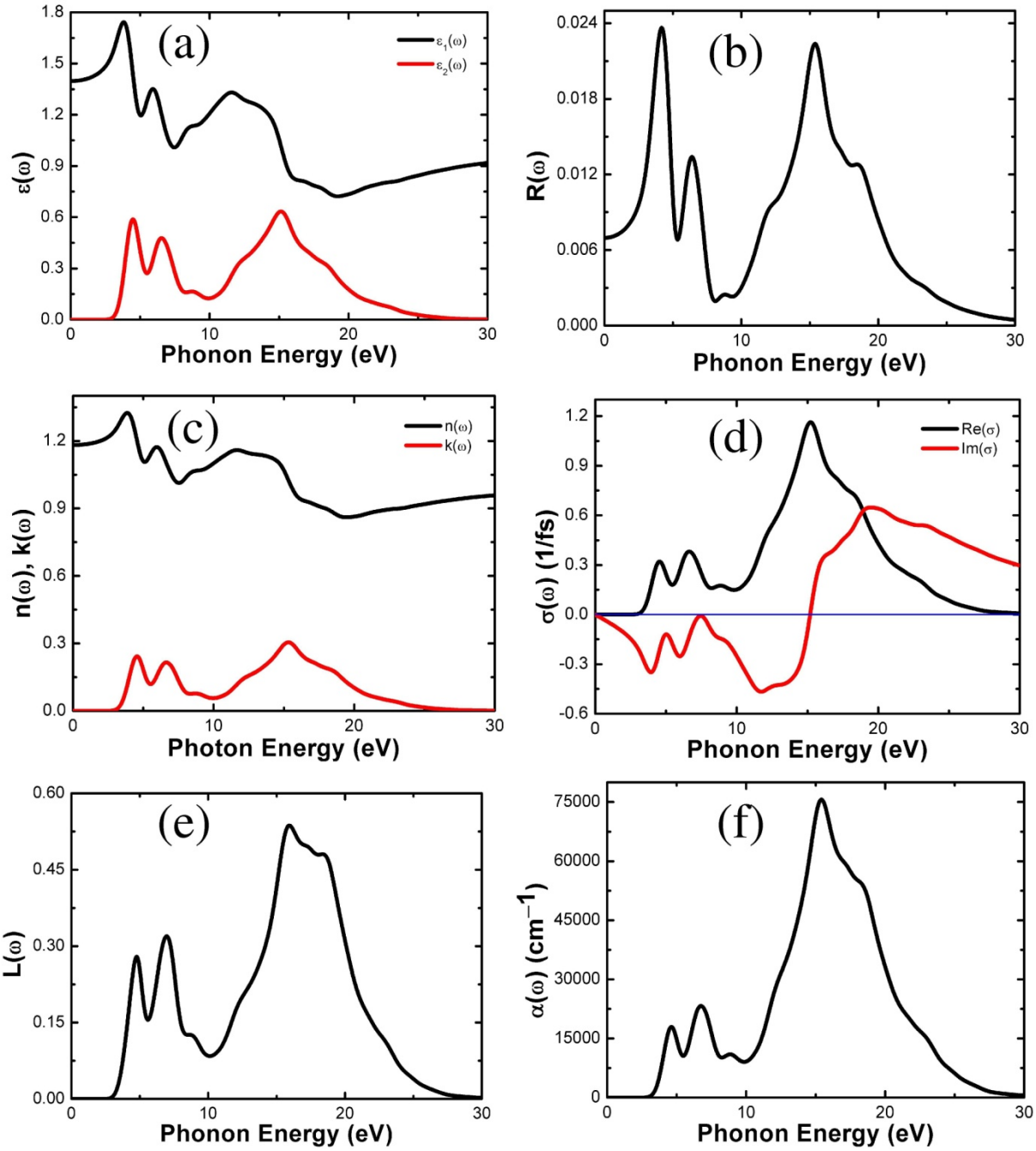

Figure S14. Calculated optical properties for Be-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

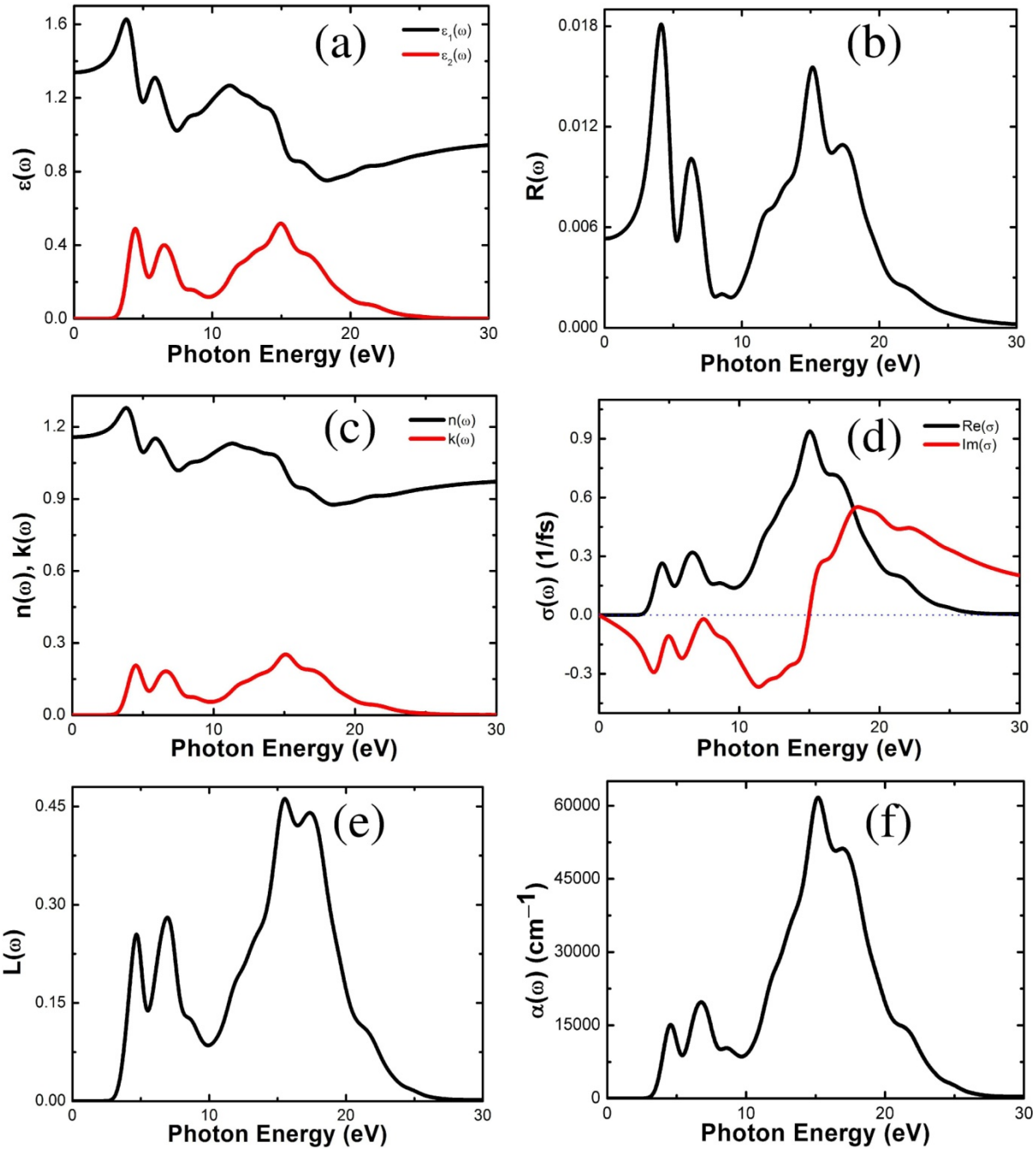

Figure S15. Calculated optical properties for Mg-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

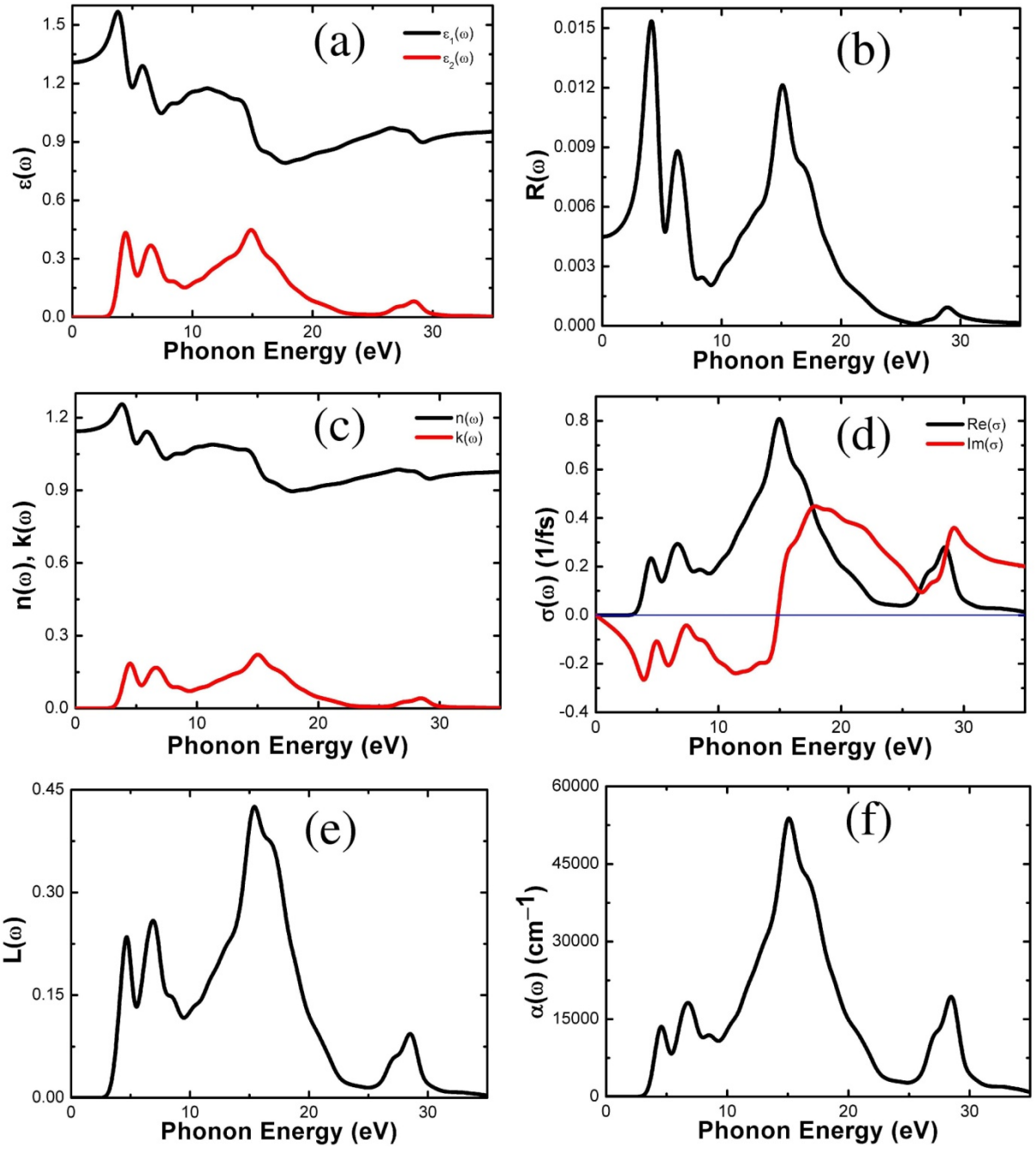

Figure S16. Calculated optical properties for Ca-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

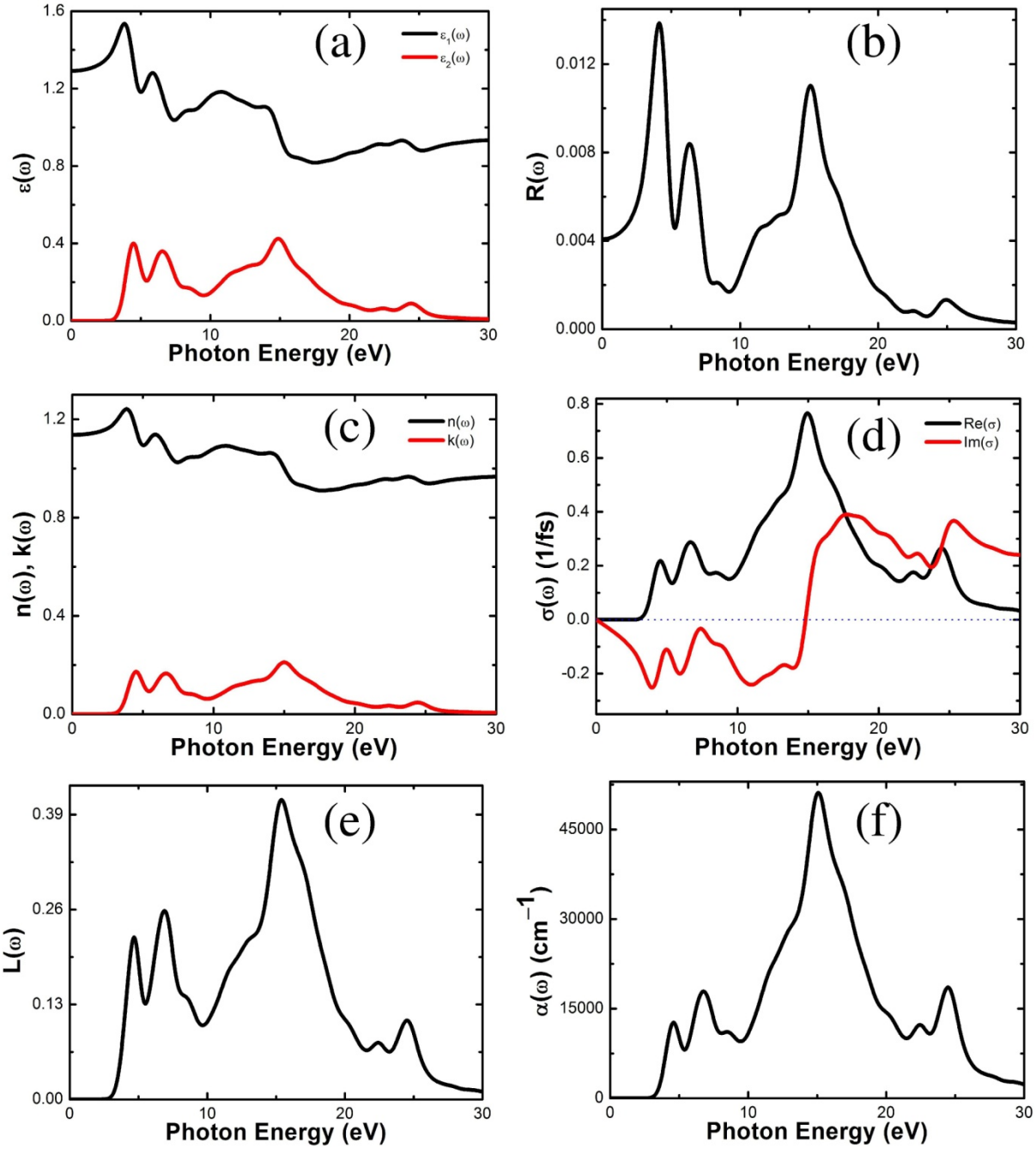

Figure S17. Calculated optical properties for Sr-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

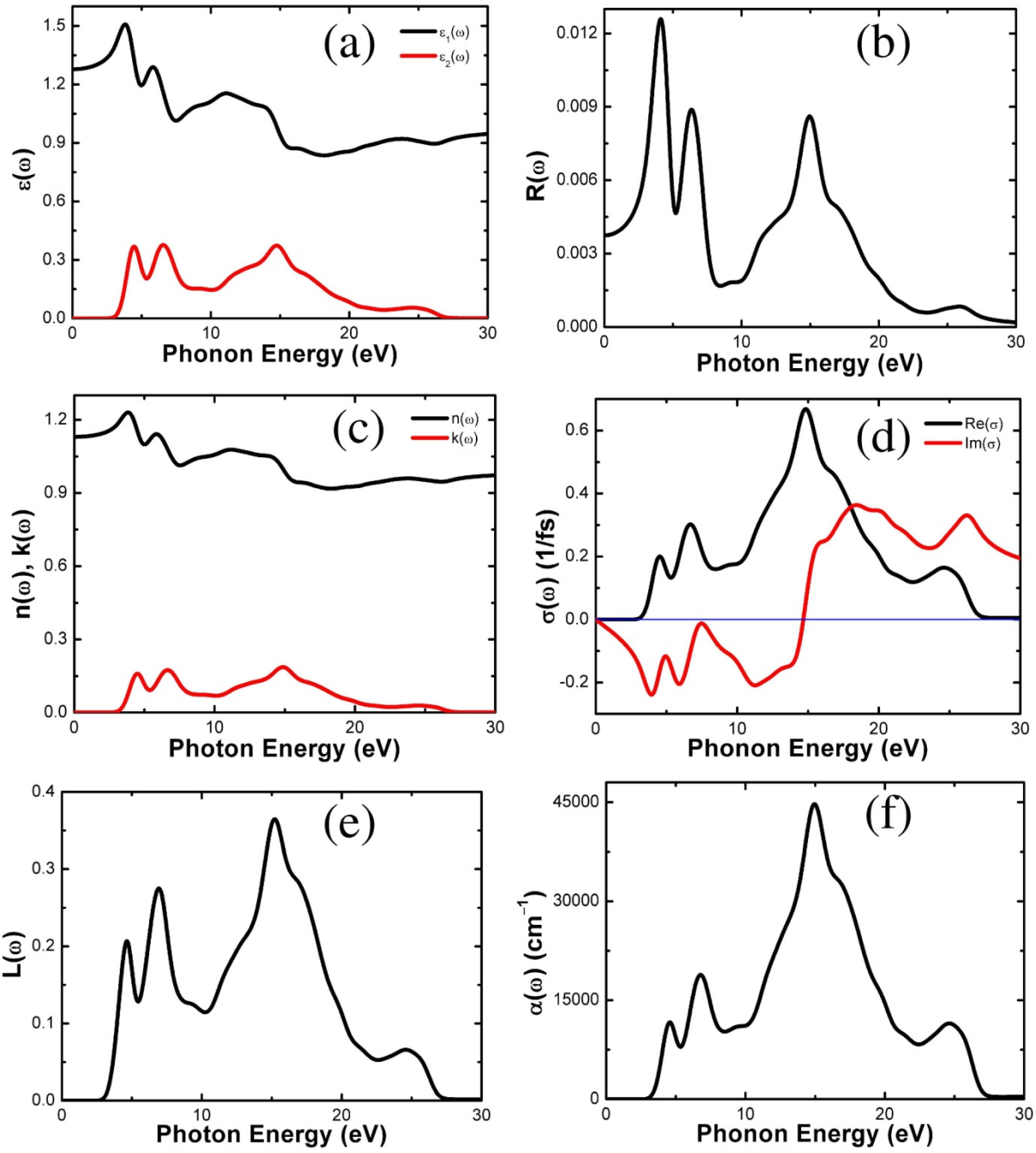

Figure S18. Calculated optical properties for Ba-IRMOF-10: (a) dielectric function ε(ω), (b) reflectivity R(ω), (c) refractive index **n**(ω); extinction coefficient **k**(ω), (d) optical conductivity σ(ω), (e) energy loss function L(ω), (f) absorption α(ω).

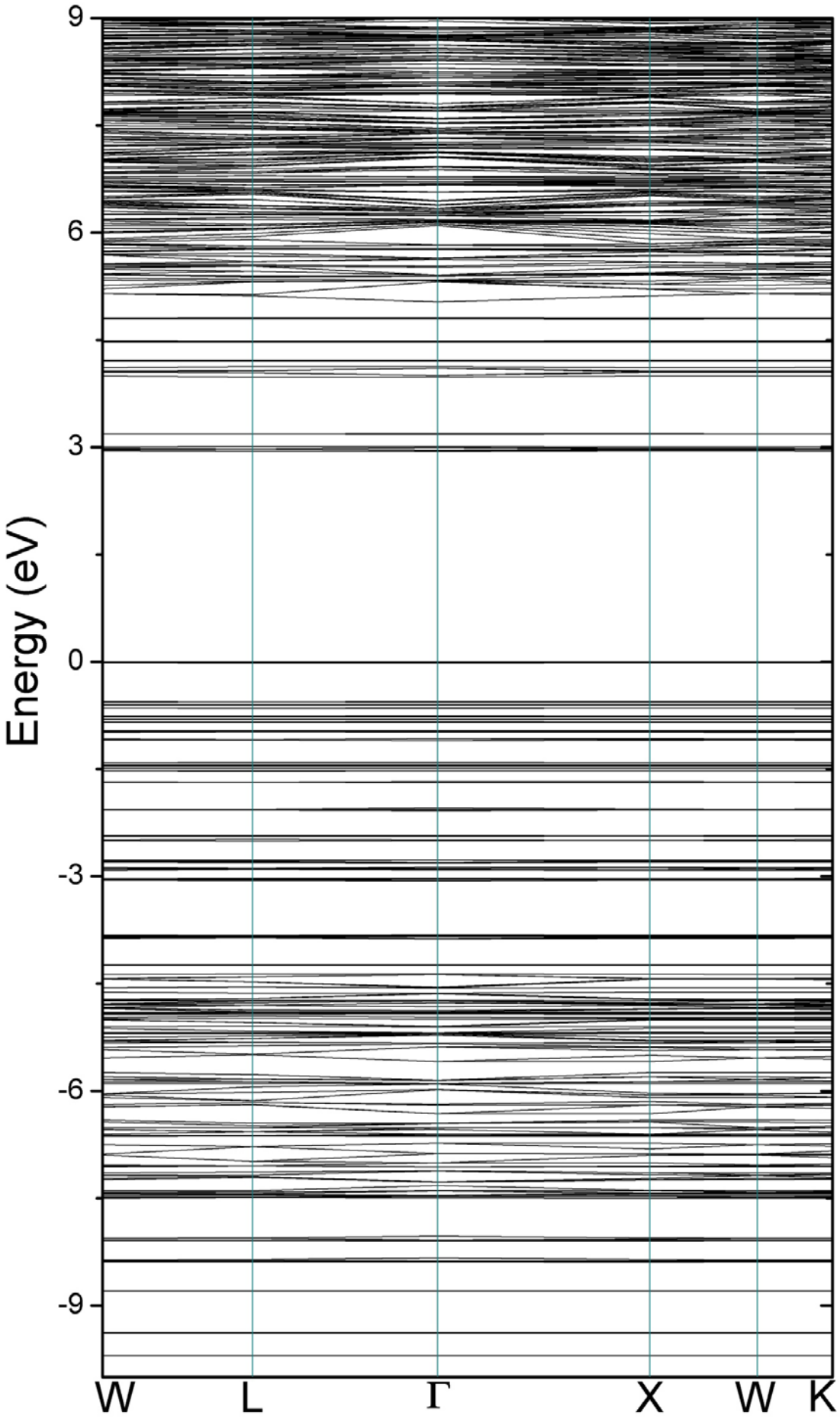

Figure S19. The electronic band structure of Cd-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

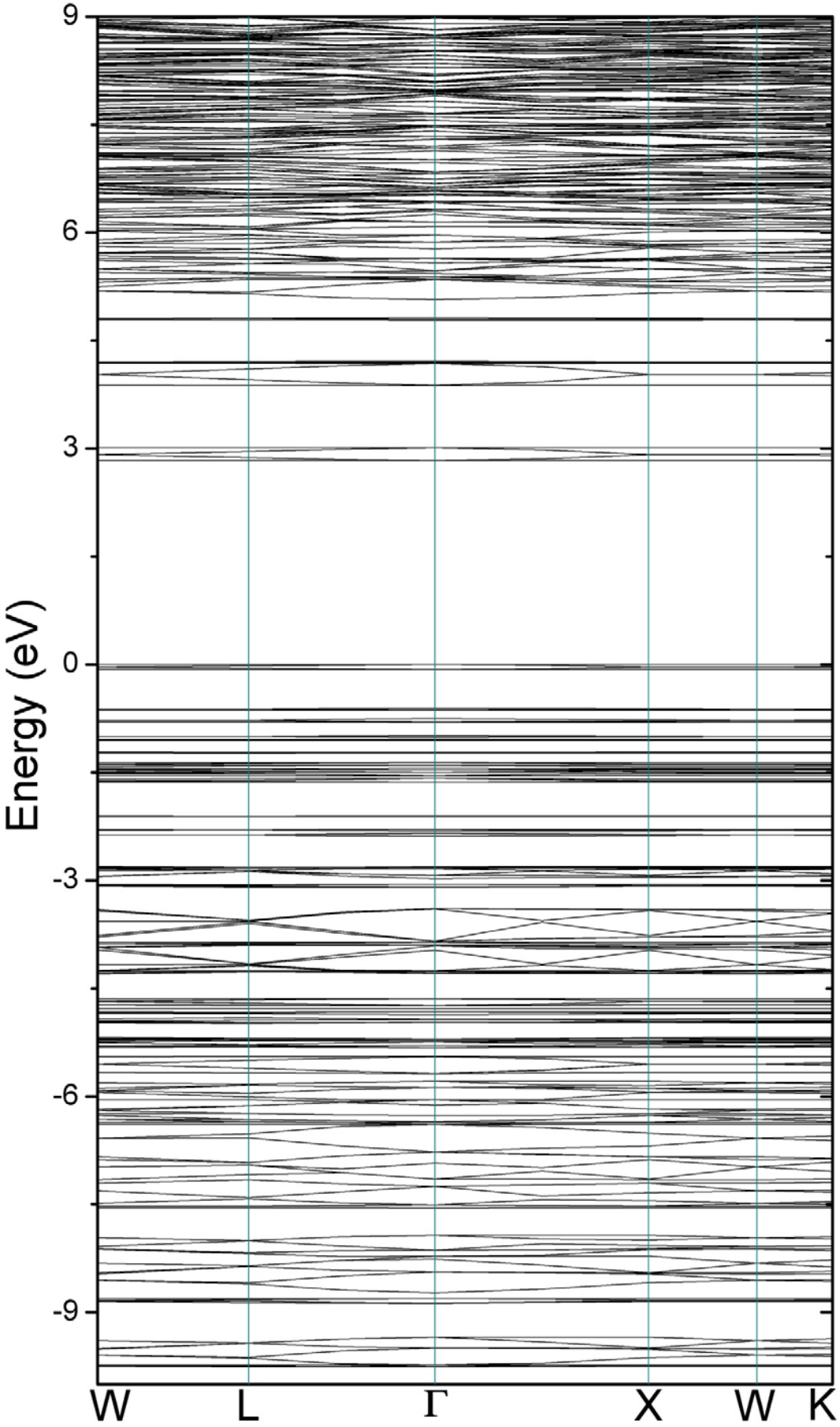

Figure S20. The electronic band structure of Be-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

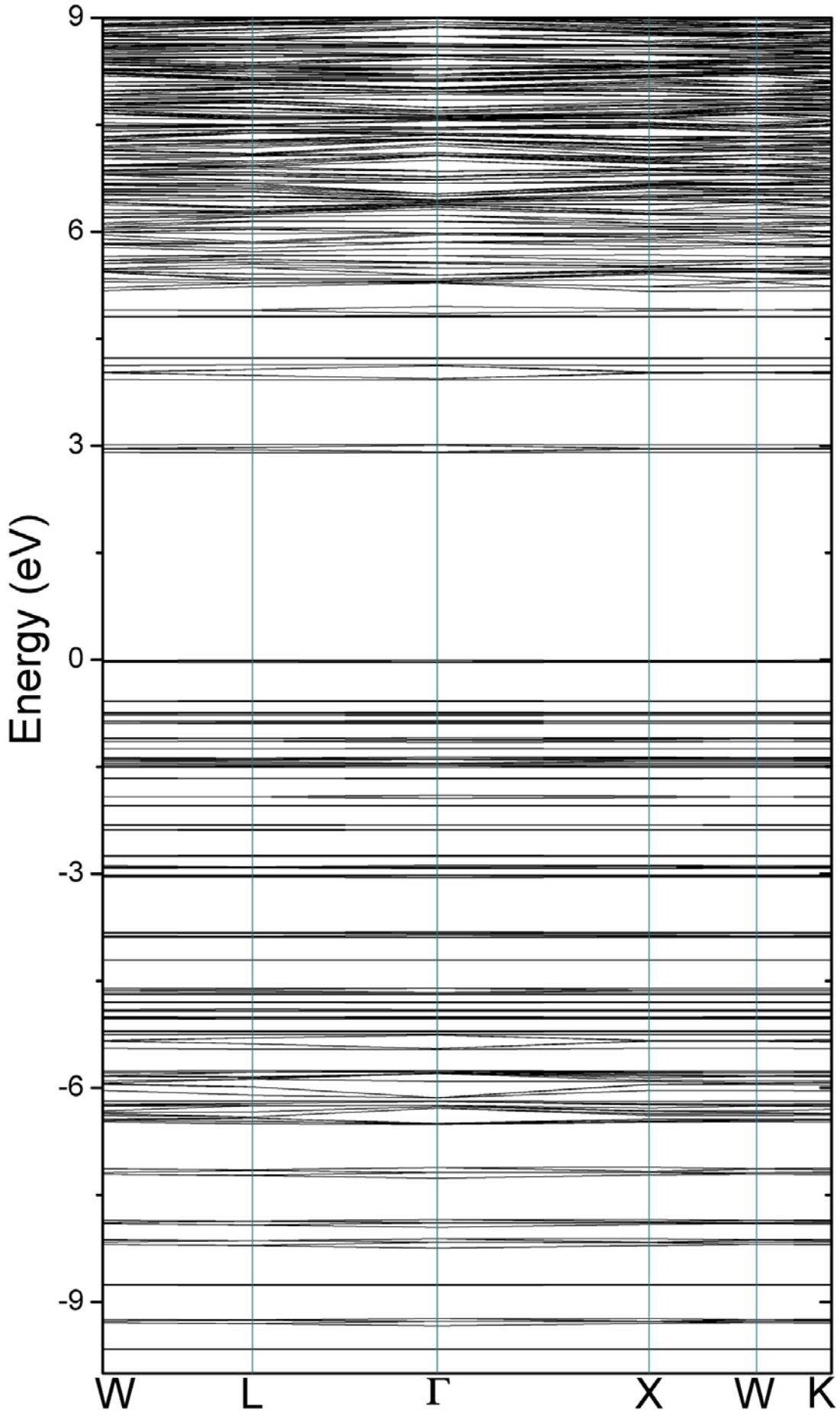

Figure S21. The electronic band structure of Mg-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

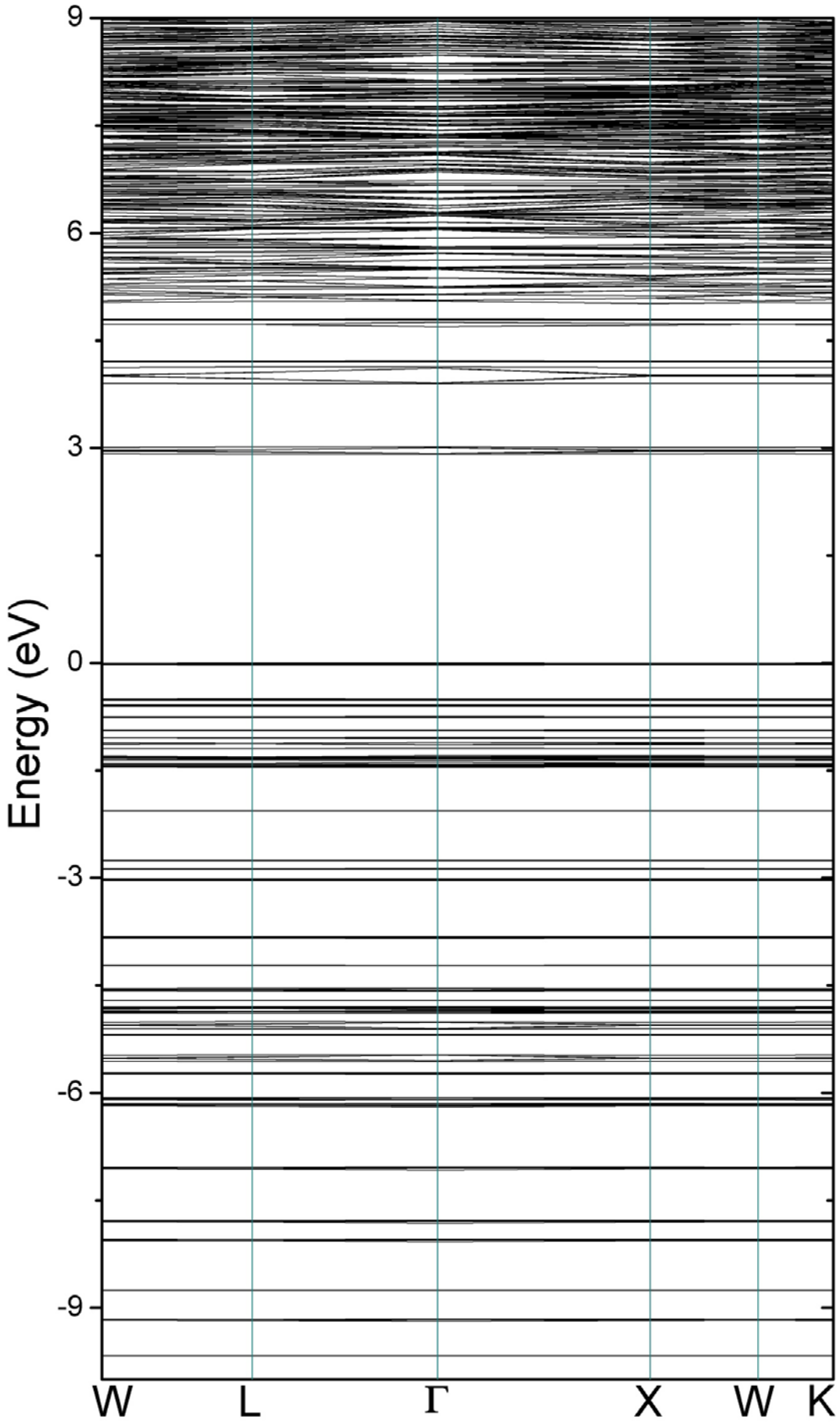

Figure S22. The electronic band structure of Ca-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

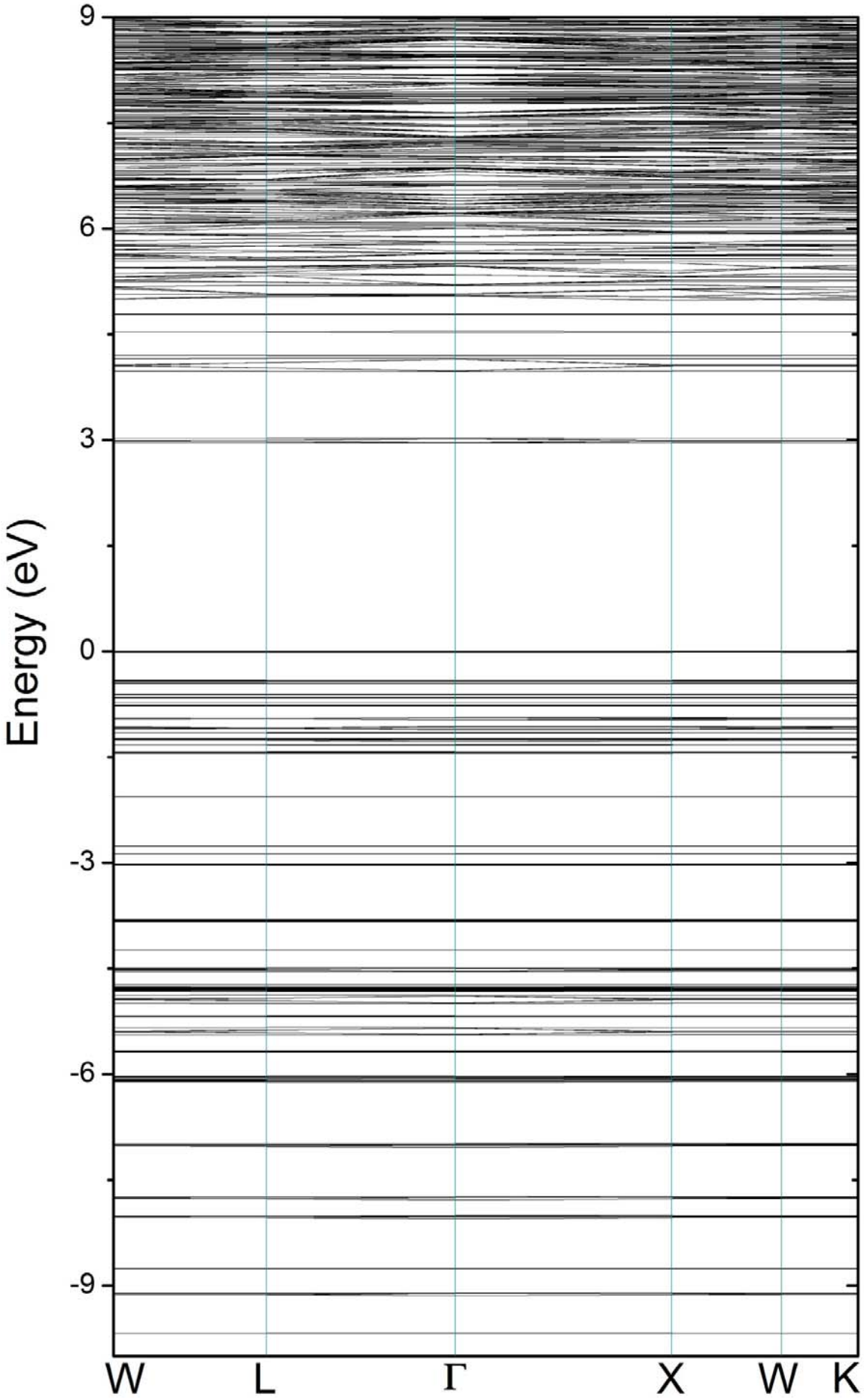

Figure S23. The electronic band structure of Sr-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.

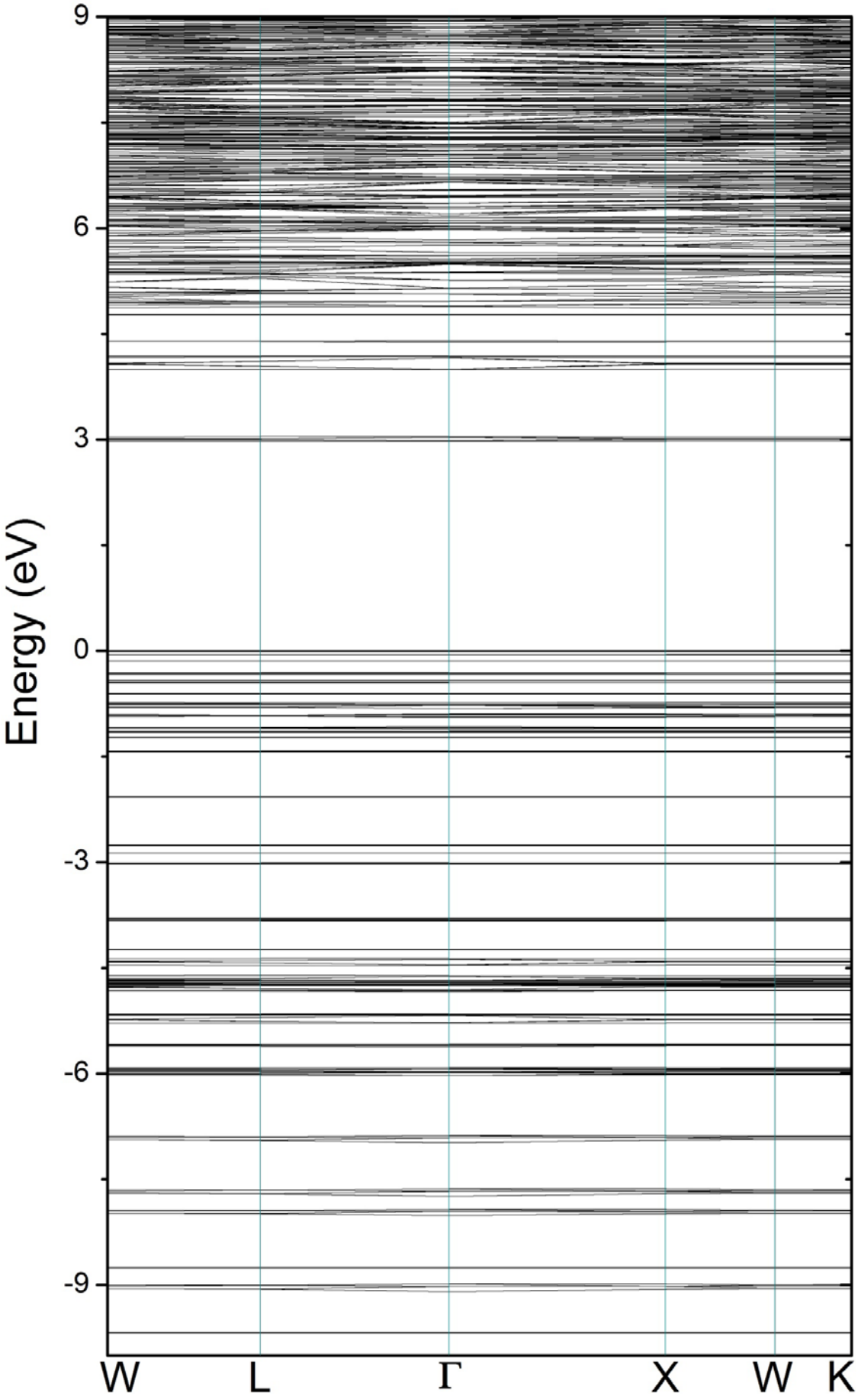

Figure S24. The electronic band structure of Ba-IRMOF-10. The Fermi level is set to zero and placed in the valence band maximum.