Supplemental Information for:

Structure and electronic properties of rare earth DOBDC metal-organic-frameworks

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Additional figures referred to in the main manuscript are included below. Data used to generate the figures below and in the main manuscript is also included as a supplemental file titled RE-MOF-Data.pdf.

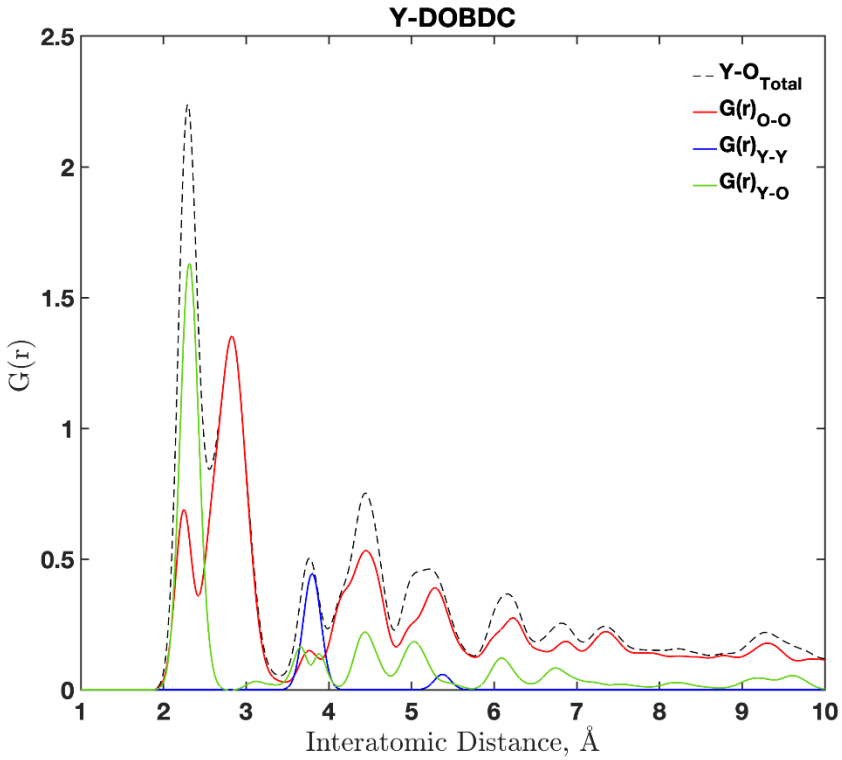

Figure S1. Composition of total pair distribution function (dashed line) of Y-DOBDC represented individually by interatomic contributions: O-O(red), Y-Y(blue), and Y-O(green).

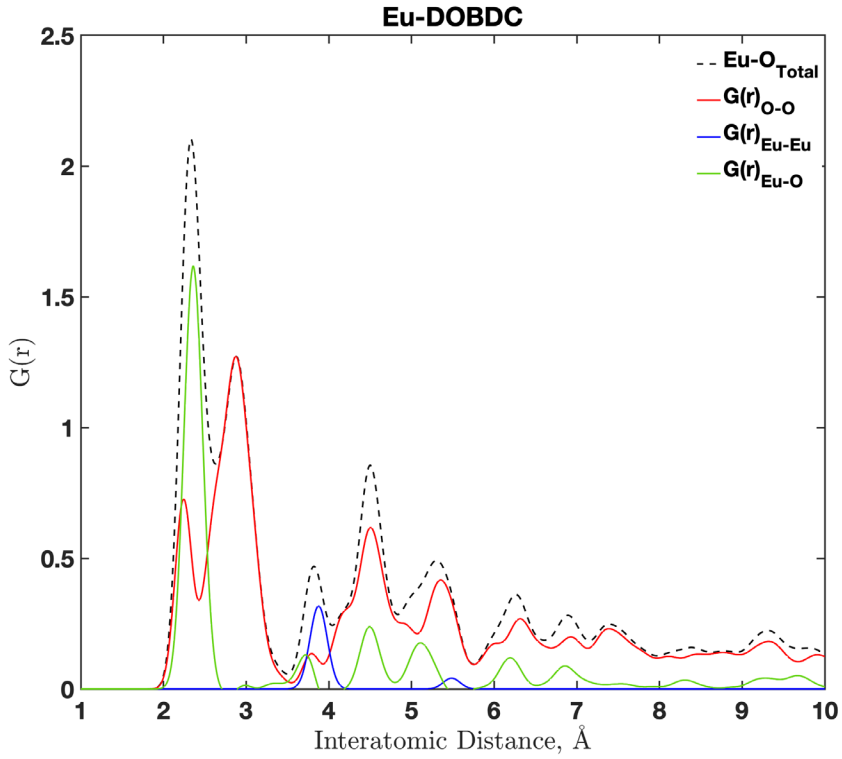

Figure S2. Composition of total pair distribution function (dashed line) of Eu-DOBDC represented individually by interatomic contributions: O-O (red), Eu-Eu (blue), and Eu-O (green).

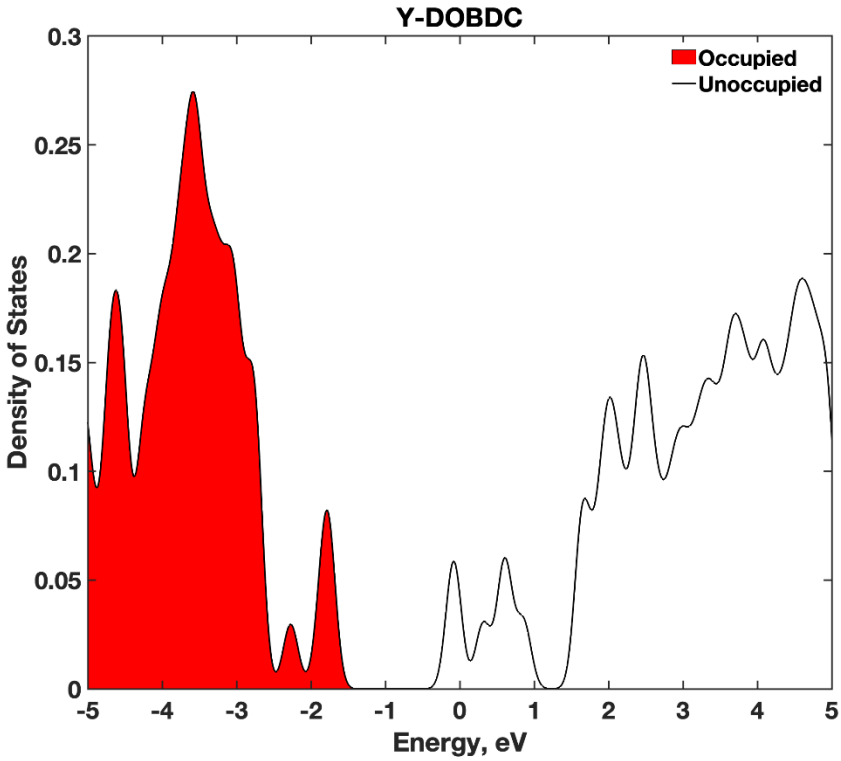

Figure S3. Density of states of Y-DOBDC. Shaded (occupied) and unshaded (unoccupied) states represent the valence and conduction bands, respectively.

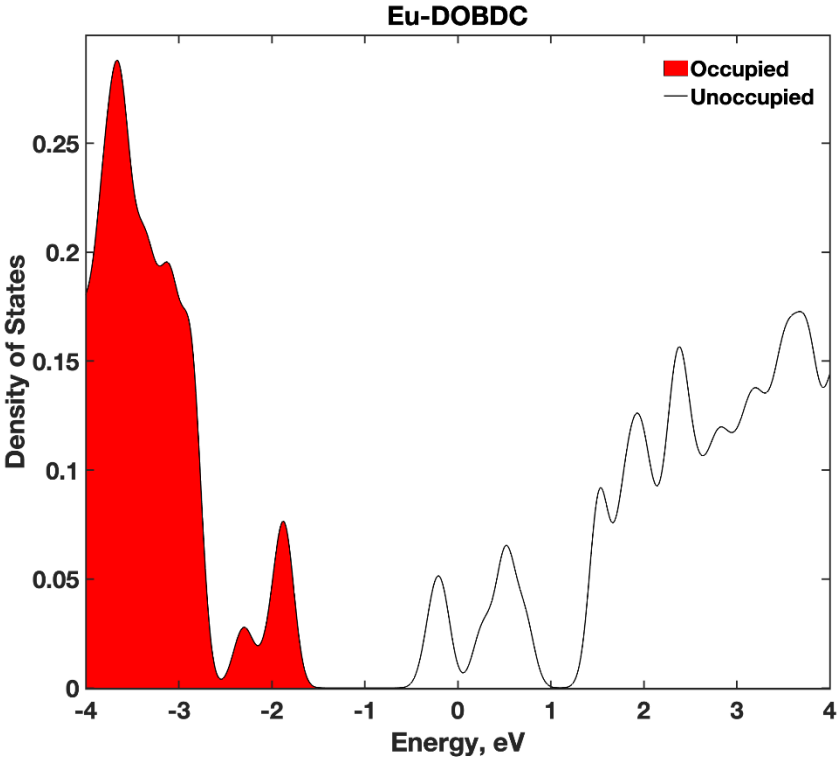

Figure S4. Density of states of Eu-DOBDC. Shaded (occupied) and unshaded (unoccupied) states represent the valence and conduction bands, respectively.

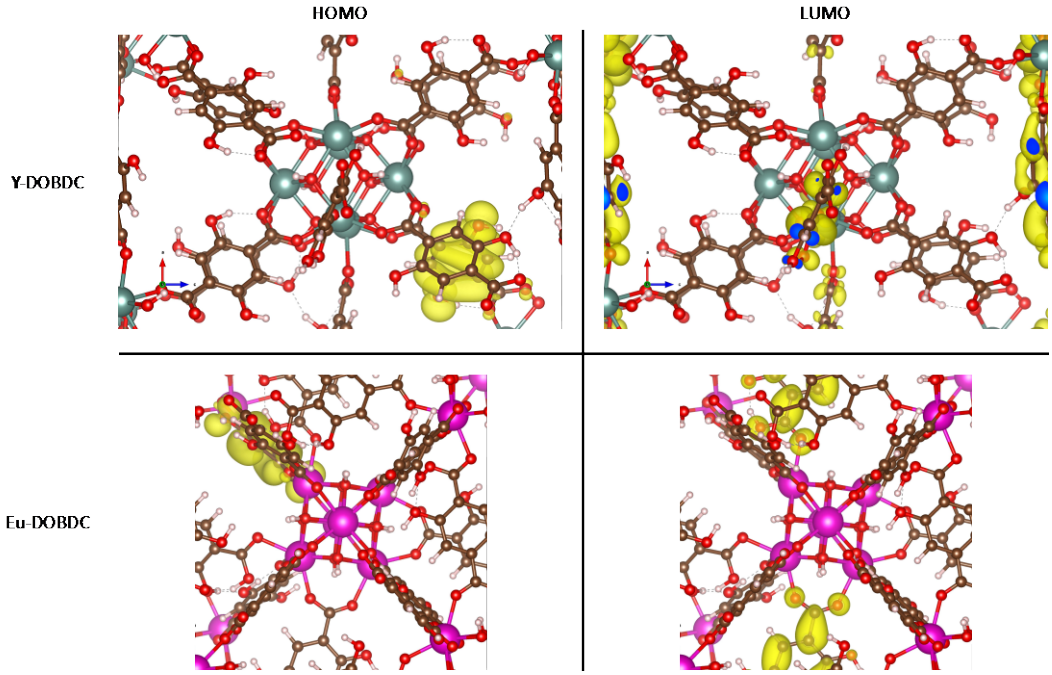

Figure S5. Partial charge densities of the highest occupied molecular orbital (HOMO, left) and lowest unoccupied molecular orbital (LUMO, right) for Y- and Eu- DOBDC. For the Y-DOBDC model (top) the elements are presented as Y(green), O(red), C(brown), and H(white). For the Eu-DOBDC model the elements are presented as Eu(pink), O(red), C(brown) and H(white). The partial charge densities are modeled as yellow isosurfaces.

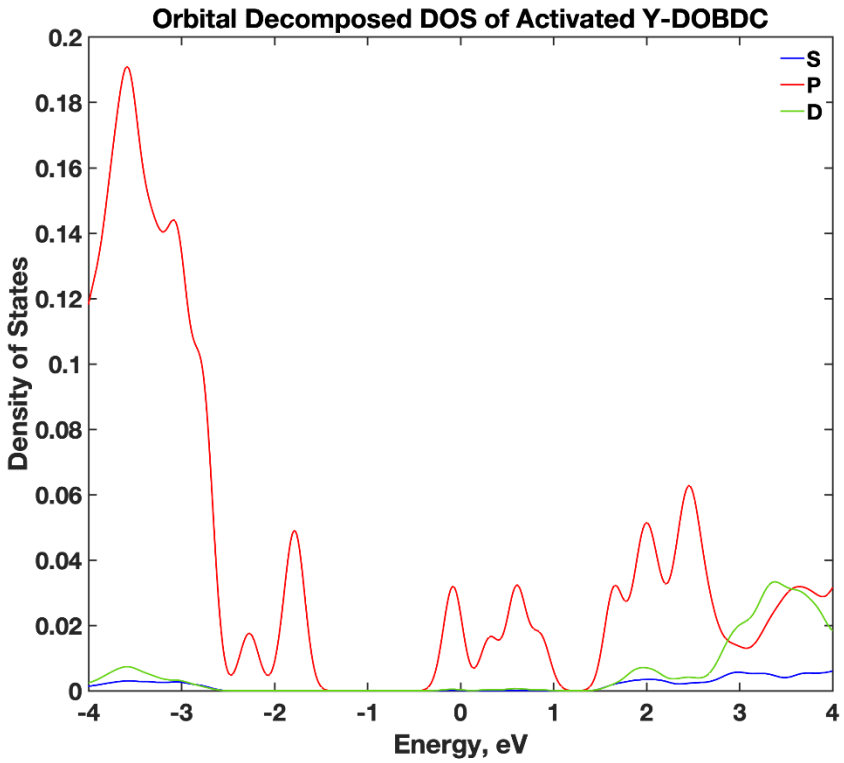

Figure S6. Orbital decomposed DOS for Y-DOBDC calculated with spin-restricted DFT.

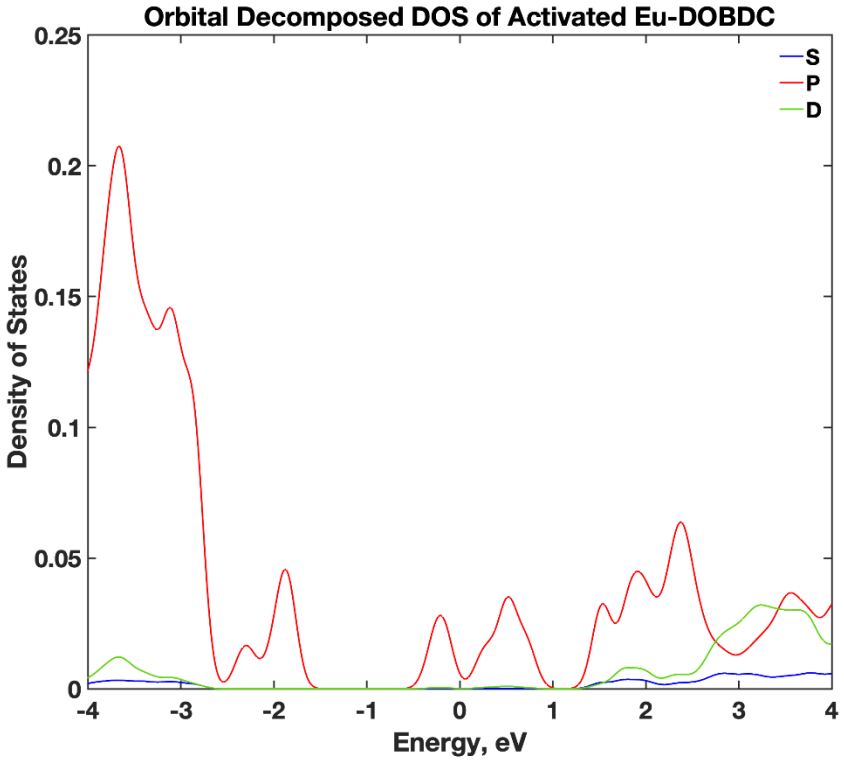

Figure S7. Orbital decomposed DOS for Eu-DOBDC calculated with spin-restricted DFT using LCPs.

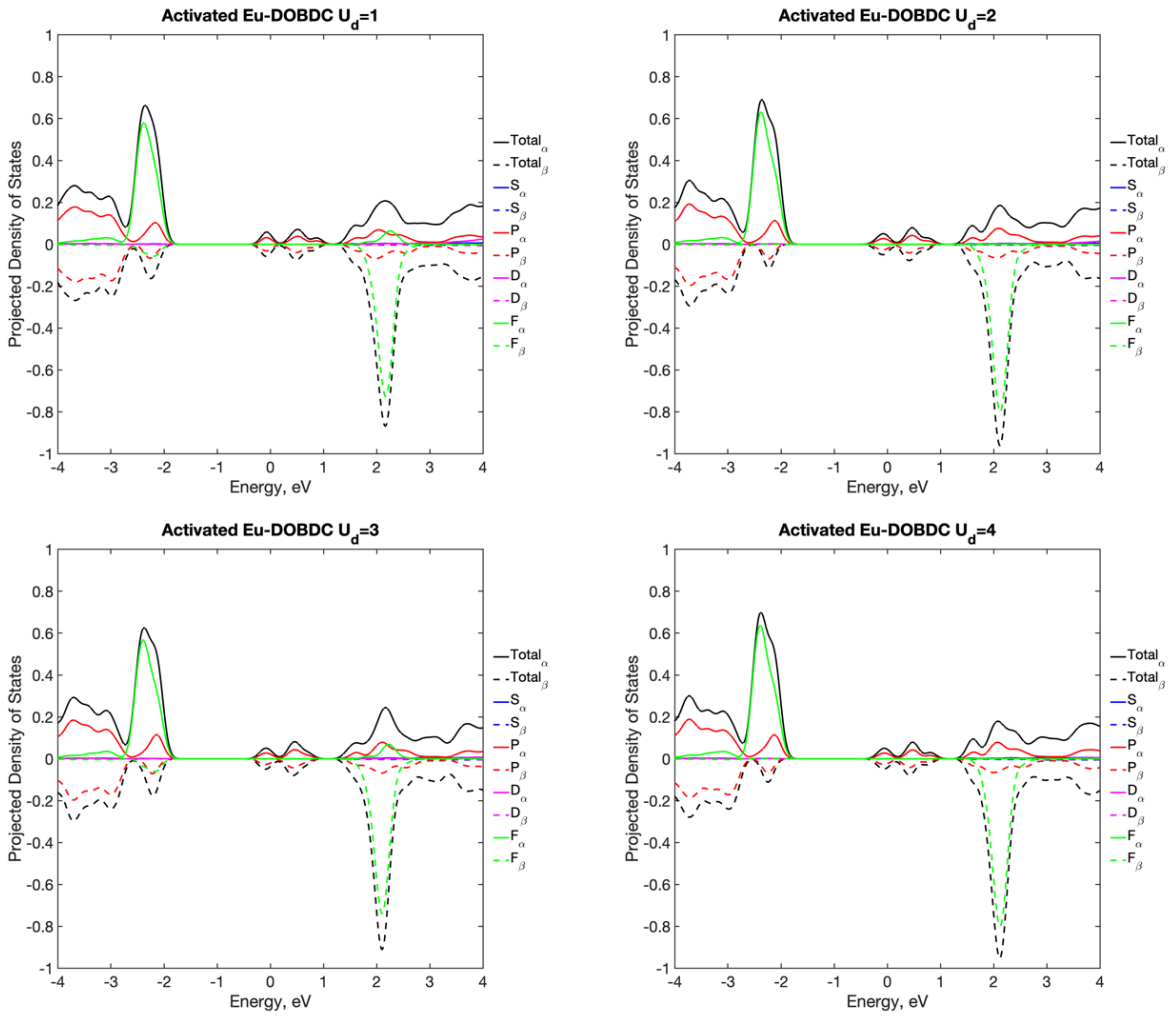

Figure S8. Projected density of states (PDOS) for activated Eu-DOBDC calculated with PBEsol-D3+U, where U=1-4. Each PDOS provides individual orbital contributions (blue, S; red, P; pink, D; green, F) to the total (black) distribution of electronic states for both the alpha (solid) and beta (dashed) spin projections. The Hubbard U values are applied to the d electrons of Eu.

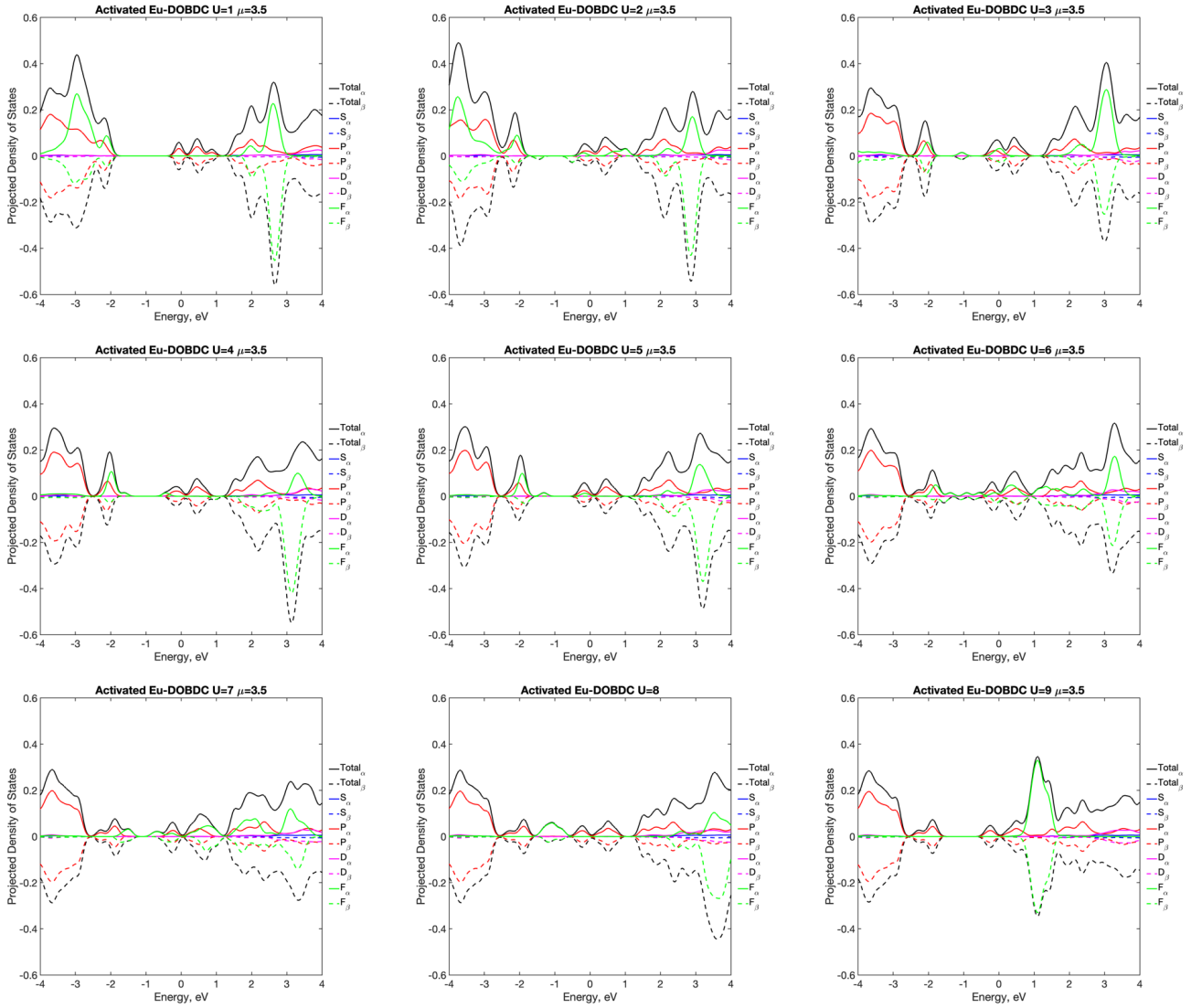

Figure S9. Projected density of states (PDOS) for activated Eu-DOBDC calculated with PBEsol-D3+U, where U=1-9. Each PDOS provides individual orbital contributions (blue, S; red, P; pink, D; green, F) to the total (black) distribution of electronic states for both the alpha (solid) and beta (dashed) spin projections. The Hubbard U values are applied to the f electrons of Eu.

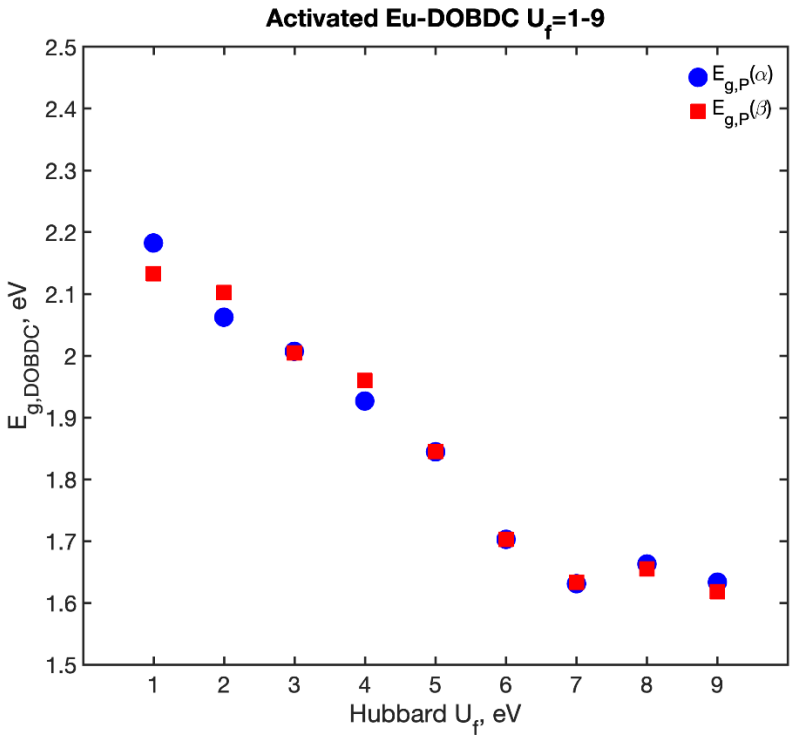

Figure S10. Band gap energies calculated for the electronic P orbital states localized on the DOBDC linkers as a function of Hubbard U correction. The DOBDC band gap show that alpha (blue circle) and beta (red square) energies are of similar magnitude for all values of U(eV)=1-9.

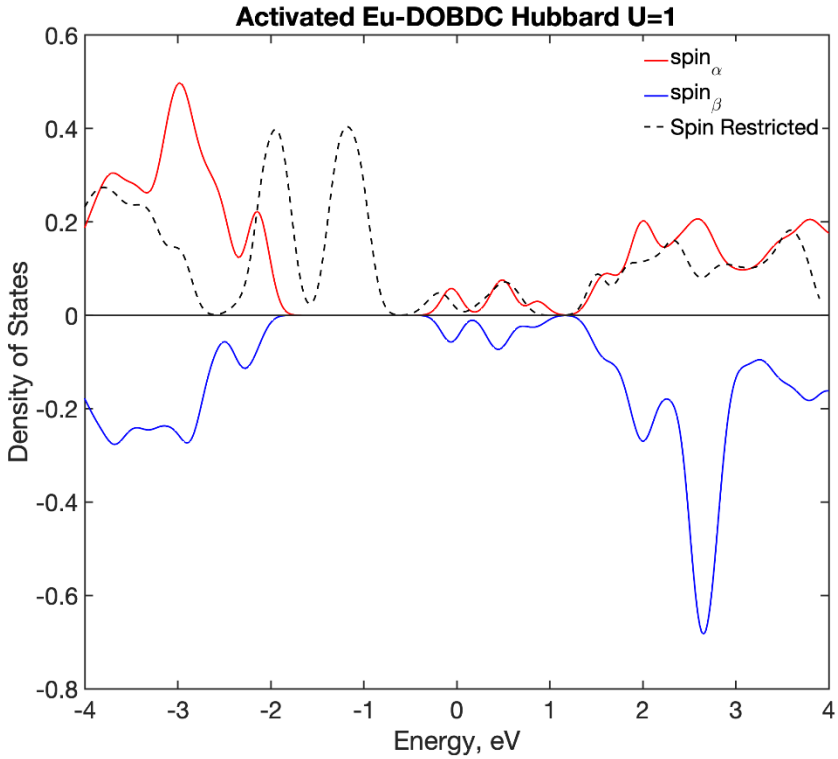

Figure S11. DOS comparison of activated Eu-DOBDC calculated with spin restricted and spin unrestricted DFT. The spin-restricted (black dashed) DOS shows a band gap that is nearly closed, whereas the spin-unrestricted (red and blue solid) DOS show the spin α and β, respectively, have an open gap to allow for expected emission.

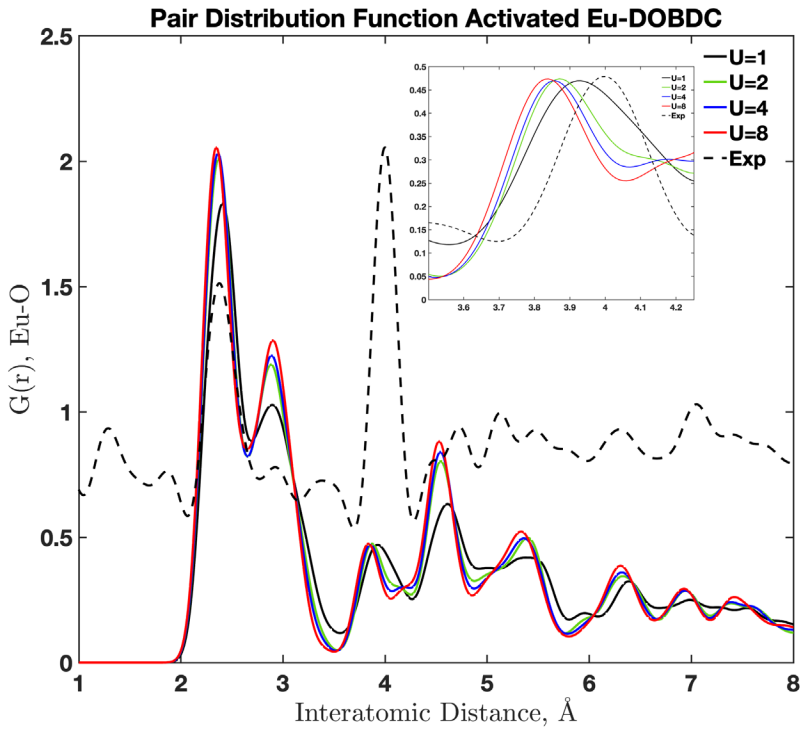

Figure S12. Eu-O bond pair distribution functions in activated Eu-DOBDC calculated with spin-unrestricted DFT with varying values of the Hubbard U correction. The values for U=1(black), 2(green), 4(blue), and 8(red) are compared with the normalized experimental value (black dashed) presented. The inset displays the calculated and normalize experimental peaks corresponding to the RE-RE peak. The calculated PDFs for U>1 show a more contracted interatomic distance.