Electronic Supplementary Information

To

Structural and electronic properties of $KY(BH_4)_4$: DFT + U study

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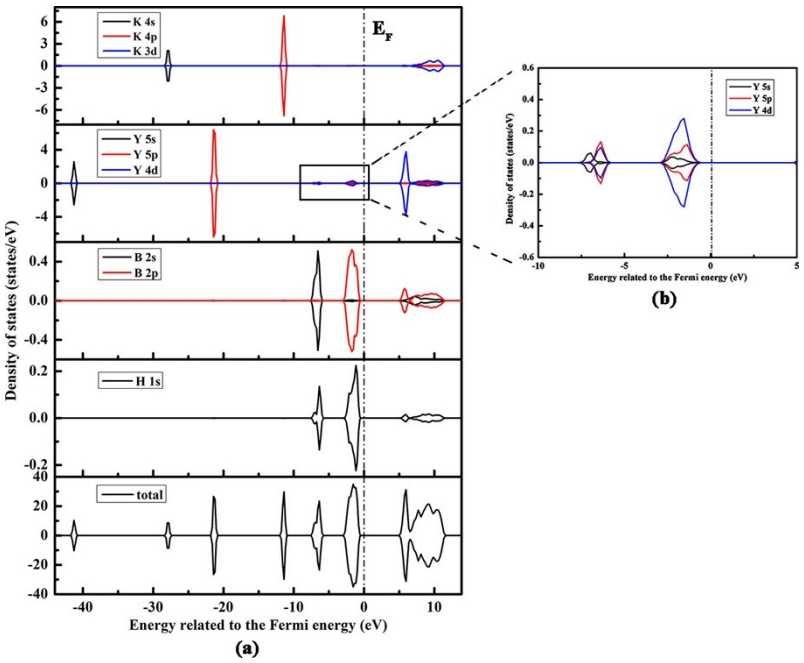

Fig. S1 The calculated total and partial density of states of $KY(BH_4)_4$ by the PBE + U method at U = 3 eV, and the Fermi energy is set to zero.

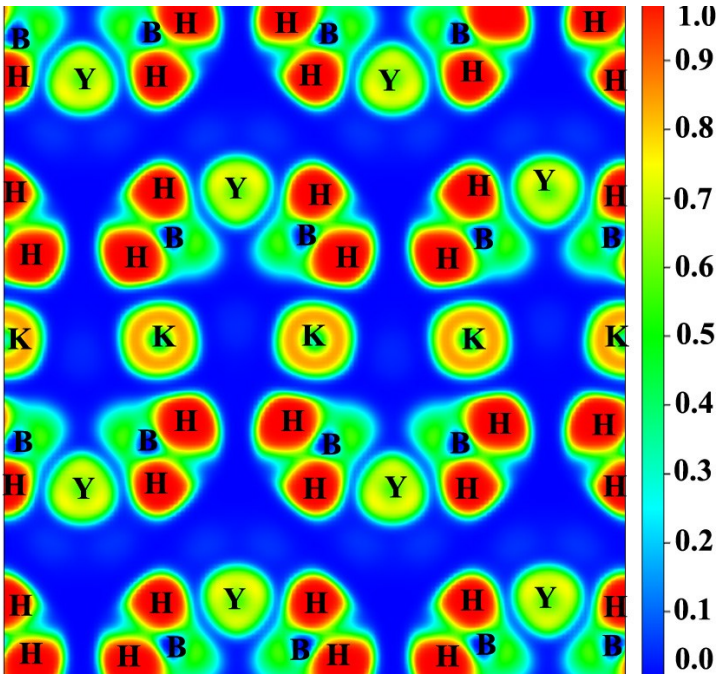

Fig. S2 The calculated ELF of $KY(BH_4)_4$ by the PBE + U method at U = 3 eV.

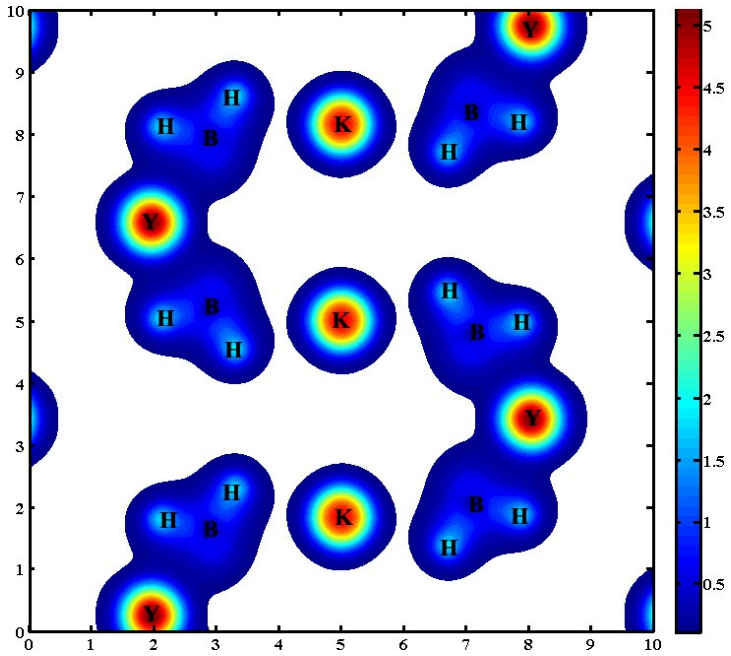

Fig. S3 The calculated total charege density of $KY(BH_4)_4$ by the PBE + U method at U = 3 eV.