Supplemental Material: Role of Lanthanide in the Electronic Properties of $RbLn_2Fe_4As_4O_2$ (Ln = Sm and Ho) Superconductors

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GGA + U is a density functional theory (DFT) computational method developed to accurately describe the electronic structure and properties of materials containing localized electrons. It incorporates a Hubbard U correction term on top of the standard GGA approximation to simulate and adjust the Coulomb interaction of localized electrons. This method is particularly useful for handling the 4f electrons in rare earth elements and the 3d electrons in transition metal materials. By introducing the Hubbard U term, the GGA + U method can better describe the magnetic, charge transfer, and ionization energy characteristics of materials. Choosing an appropriate U value is crucial for the accuracy of the computational results.

I. CALCULATION OF 4F ELECTRON OF RARE-EARTH ELEMENTS SM AND HO WITH U CORRECTION

Due to the strong correlation effect of 4f electrons in rare-earth elements Sm and Ho, neglecting the U correction would lead to computational results that do not agree with experimental findings. However, since $RbSm_2Fe_4As_4O_2$ and $RbHo_2Fe_4As_4O_2$ are newly discovered materials, there are currently no available experimental data for reference. Therefore, in determining the value of U, we can only rely on previous studies and experiences to make estimations and inferences within a limited range. The range provided in references[1–5] suggests that selecting a U value between 6 eV and 12 eV is relatively reasonable. Hence, we performed U-corrected calculations for the 4f electrons of Sm and Ho within this range, and observed the results for U = 6 eV, 9 eV, and 12 eV, as shown in Fig.1 and Fig.2. Based on the results in figures, we chose U = 9 eV as an example in the main text, as this selection does not impact the overall physical conclusions.

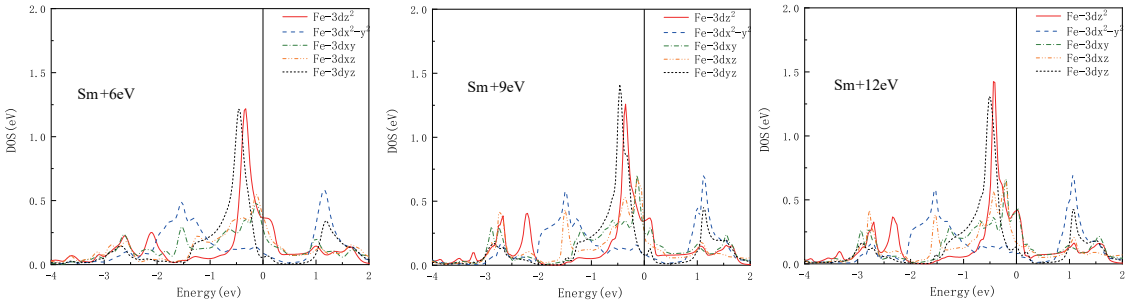

FIG. 1. (Color online) Calculation results of applying different U values to Sm's 4f electrons in $RbSm_2Fe_4As_4O_2$.

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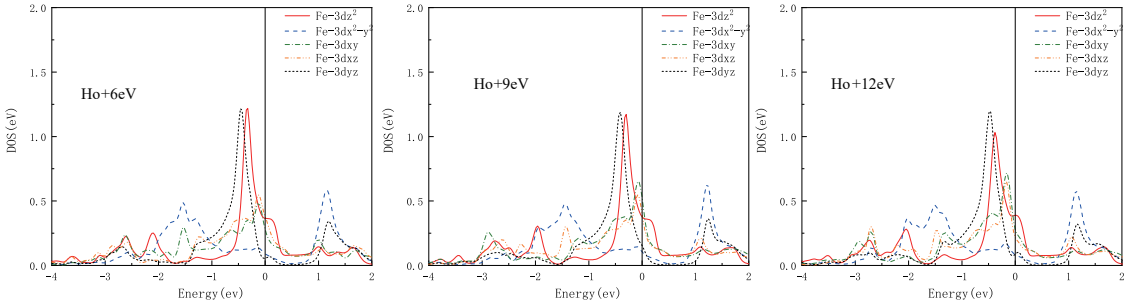

FIG. 2. (Color online) Calculation results of applying different U values to Ho' s 4f electrons in $RbHo_2Fe_4As_4O_2$.

II. CALCULATION OF 3D ELECTRON OF FE WITH U CORRECTION

The 3d electrons of iron generally exhibit strong itinerancy and Coulomb screening effects, with U values typically ranging from 0 eV to 3 eV. Based on the values provided in reference[6–10], we applied U corrections to the 3d electrons of iron with U values of 0 eV, 2 eV, and 3 eV for comparison. By comparing the results in Fig.3 and Fig.4, we found that applying the U correction does not impact the final physical conclusions.

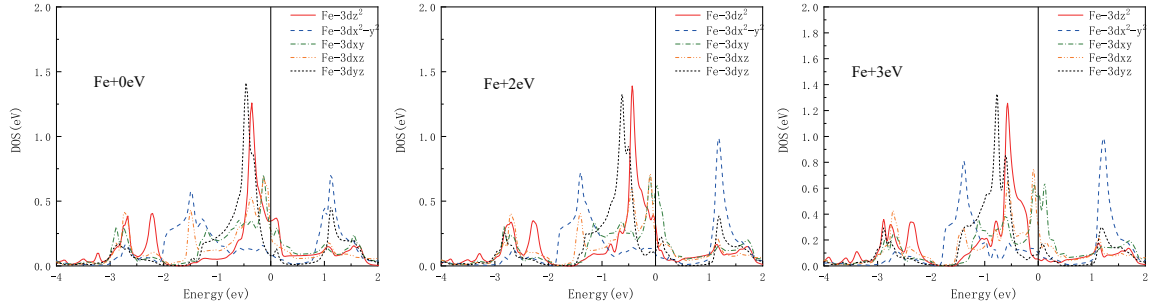

FIG. 3. (Color online) Calculation results of applying different U values to Fe' s 3d electrons in $RbSm_2Fe_4As_4O_2$.

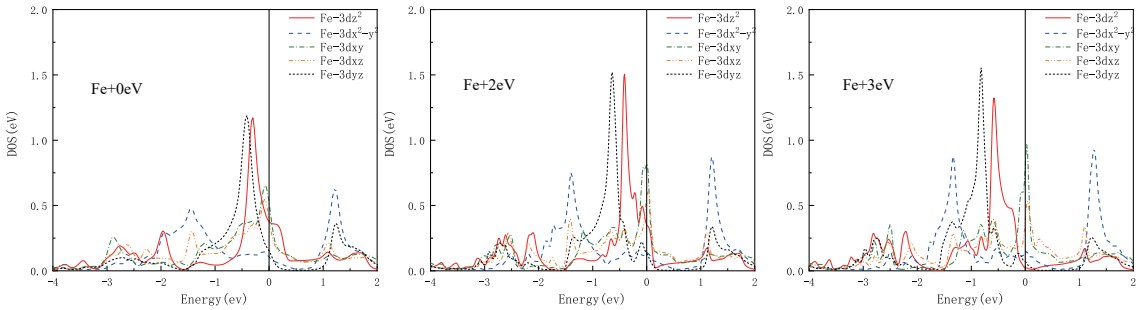

FIG. 4. (Color online) Calculation results of applying different U values to Fe' s 3d electrons in $RbHo_2Fe_4As_4O_2$.

Therefore, in the main text, we chose to apply U = 0 eV correction to the 3d electrons of iron, which does not

compromise the reliability of the calculation results..

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