Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Li doping kagome spin liquid compounds

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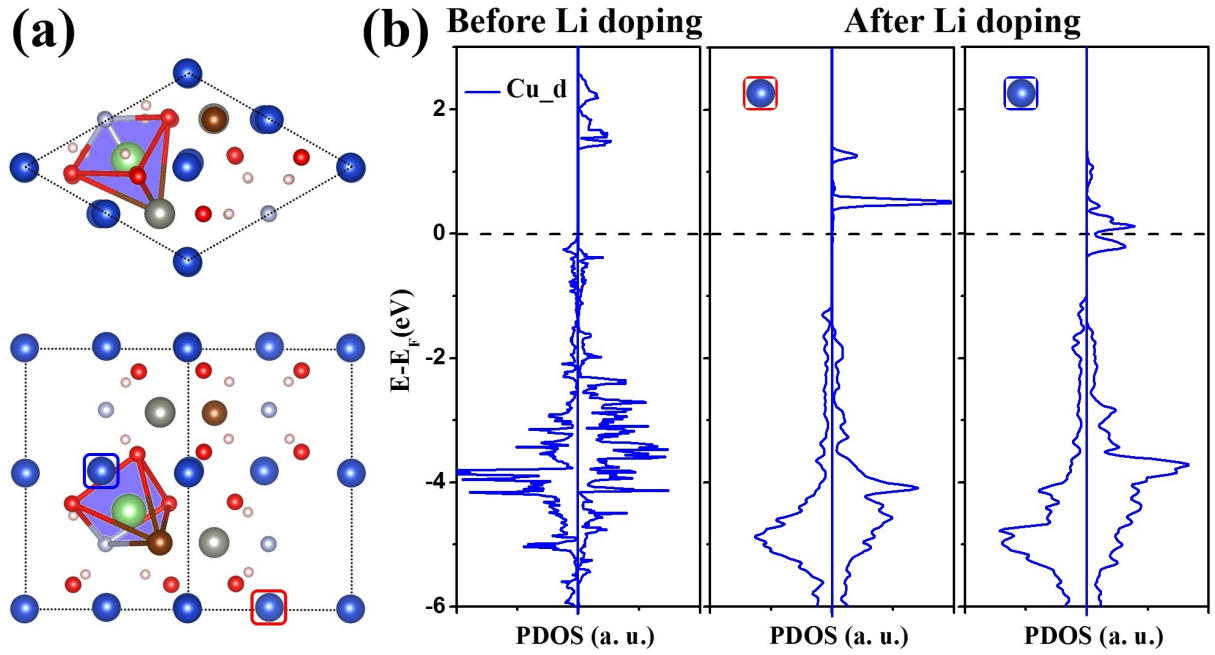

Fig. S1. Li-doped Zn-doped barlowite. (**a**) Top and side view of the most stable structure configuration for Li in Zn-doped barlowite. The Cu ions in red and blue squares represent Cu ions that are unaffected and affected by the doped Li, respectively. (**b**) PDOS of Cu ions before and after the Li doping.

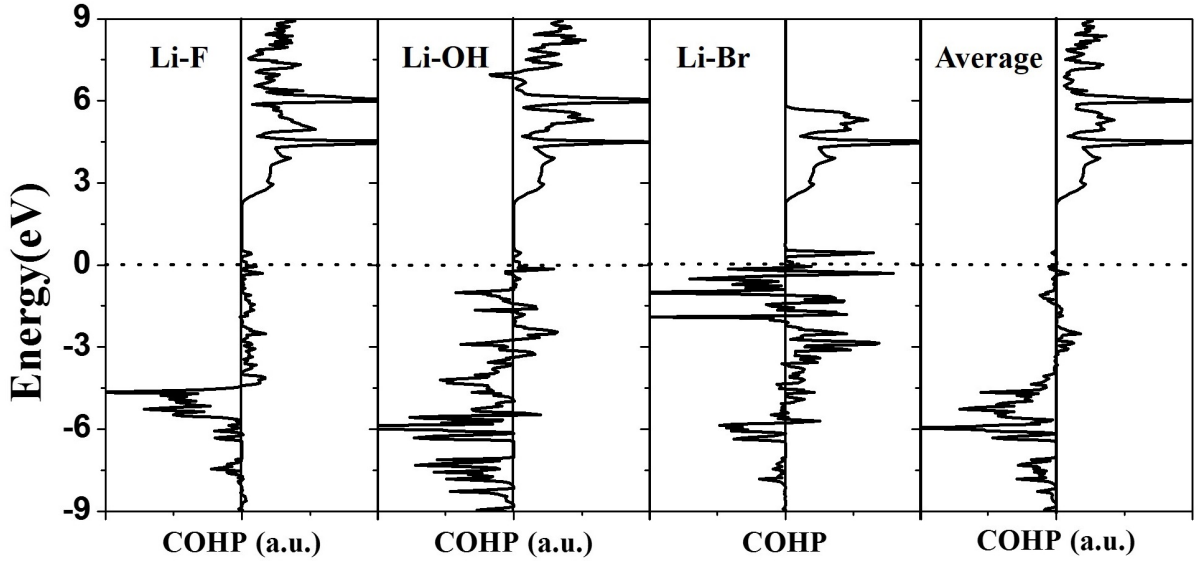

Fig. S2. Chemical bonding in Li-doped Zn-doped barlowite. COHP curve of the Li-F, Li-O, Li-Br bonds and their averaged value.

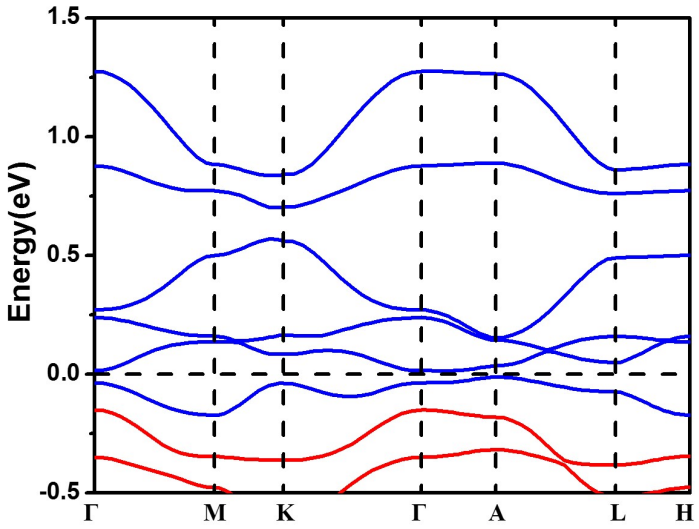

Fig. S3. Bandstructure of Li-doped Zn-doped barlowite.

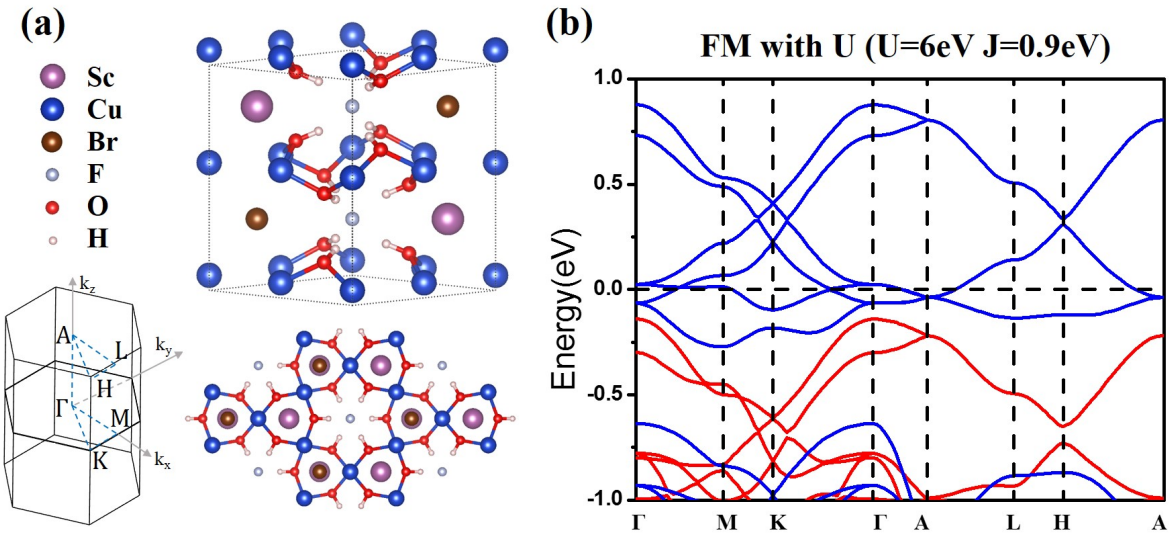

Fig. S4. Bandstructure of barlowite with element substitution of Zn with Sc. (**a**) Structure of the $ScCu_3(OH)_6BrF$. (**b**) Electronic bandstructure of $ScCu_3(OH)_6BrF$ with ferromagnetic spin configuration using on-site Hubbard U correction (U=6 eV, J=0.9 eV).