SUPPORTING INFORMATION FOR

Electronic structure and magnetic coupling of pure and Mg-doped $KCuF_3$

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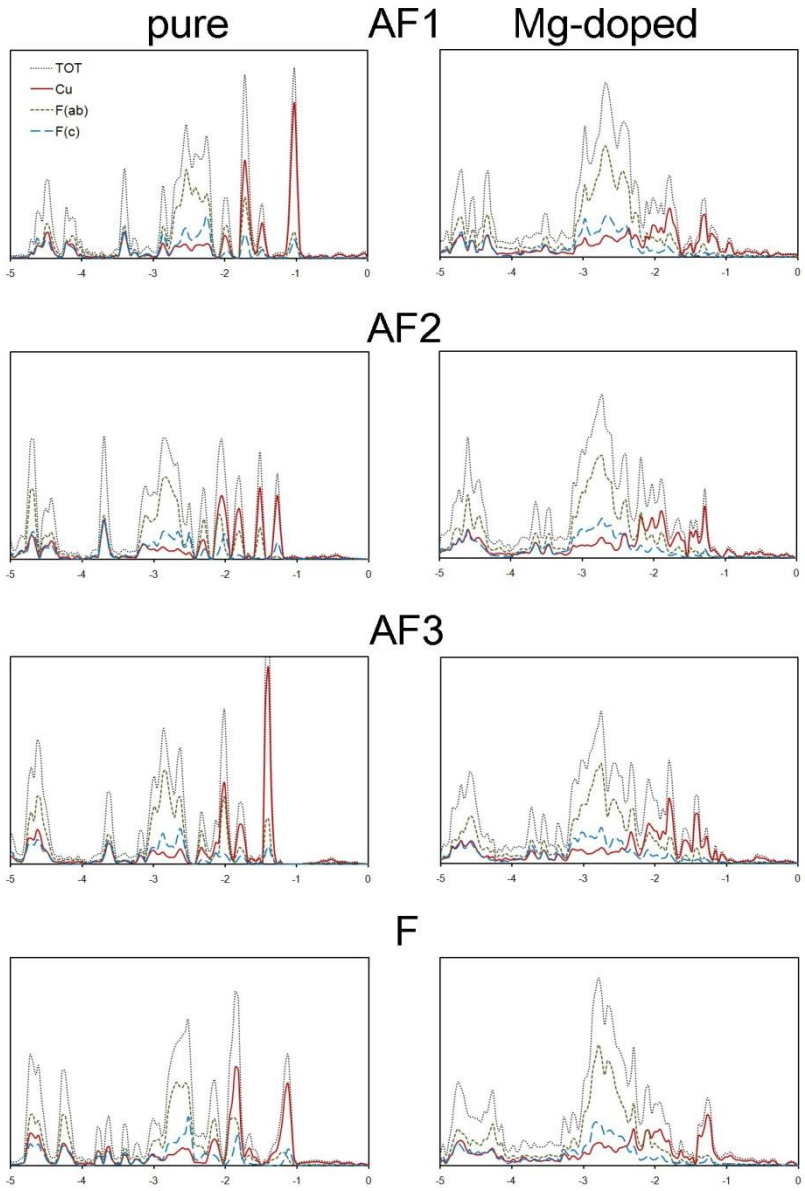

FIGURE 1SI. Total and projected DOS of pure (left) and Mg doped (right) $KCuF_3$. The Fermi level is set to zero. No relevant contribution from K and Mg is present in the energy range of the plots.

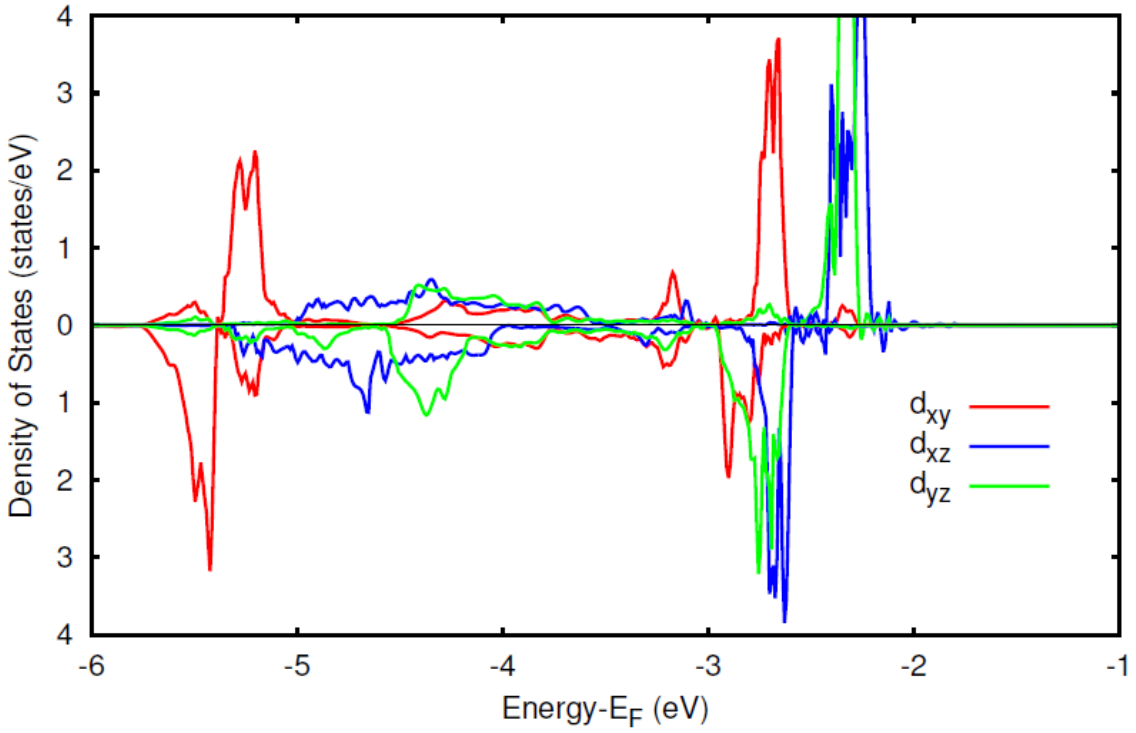

FIGURE 2SI. Projected density of states on copper atoms of pure $KCuF_3$ determined at the B3LYP level of theory for the AF1 phase for the d_{xy} (red line), d_{xz} (blue line) and d_{yz} (green line) orbitals.

Table 1SI. Magnetic coupling parameters between Cu pairs in *ab* planes (J_{ab}) and along the *c* axis (J_c) determined with the BECKE and LYP exchange and correlation functionals, respectively, without any Hartree-Fock exchange contribution.

Material	Transition	J_{ab} (K)	J_c (K)
$KCuF_3$	F - AF1		-3079
$KCuF_3$	AF2 - AF3		-1373
$KCuF_3$	AF1 - AF3	1021	
$KCuF_3$	F - AF2	737	

Table 2SI. Magnetic coupling parameters between Cu pairs in *ab* planes (J_{ab}) and along the *c* axis (J_c) determined with the BECKE and LYP exchange and correlation functionals, respectively, with a 40% Hartree-Fock exchange contribution.

Material	Transition	J_{ab} (K)	J_c (K)
$KCuF_3$	F - AF1		-150
$KCuF_3$	AF2 - AF3		-212
$KCuF_3$	AF1 - AF3	10	
$KCuF_3$	F - AF2	-39	