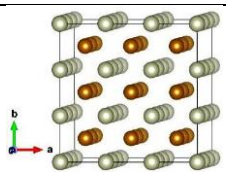
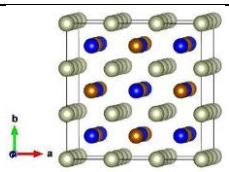
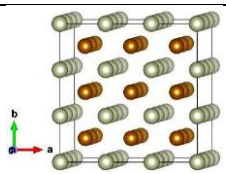
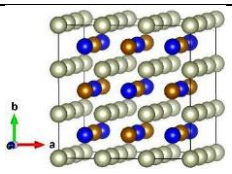
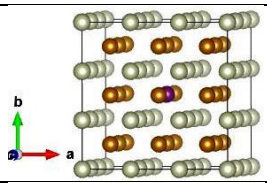
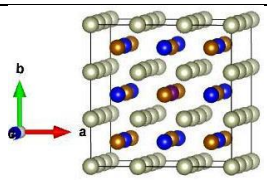
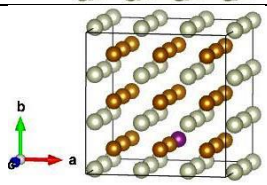
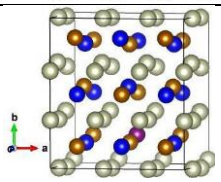
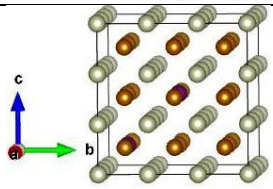
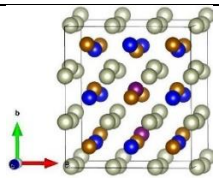
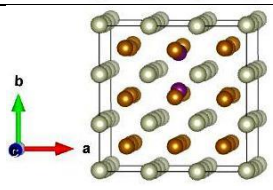
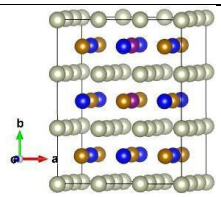
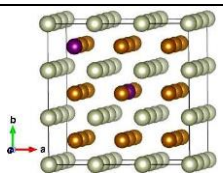
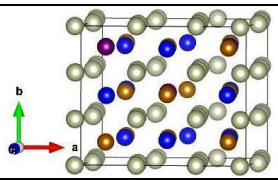
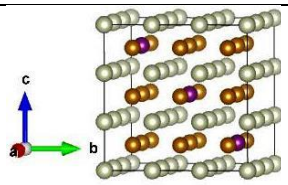
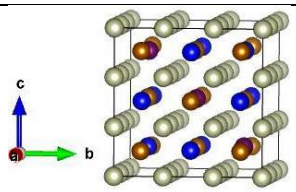
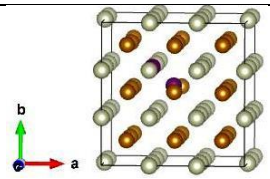
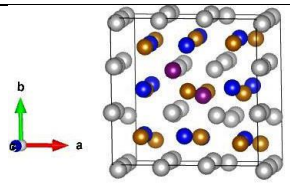
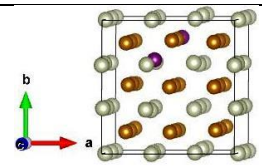
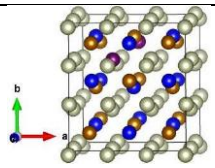
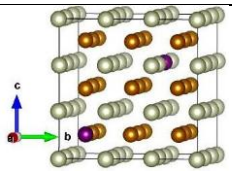
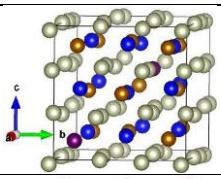
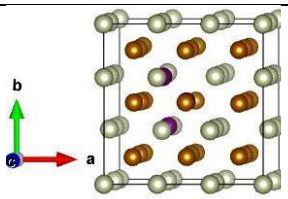
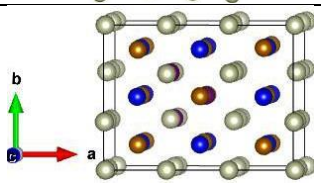
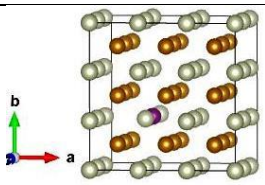
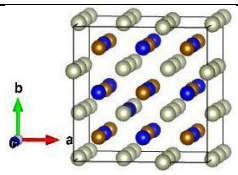
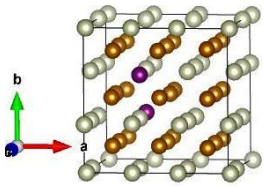
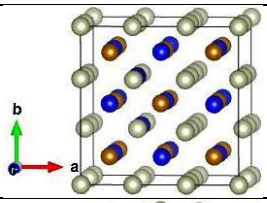
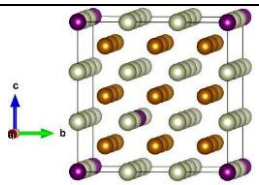
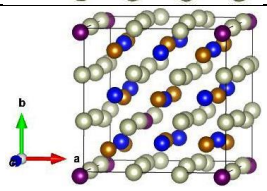
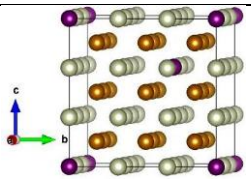
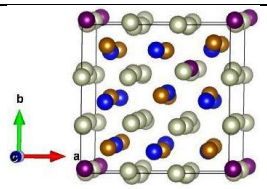
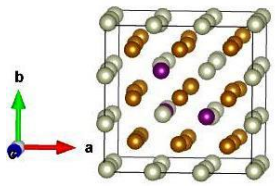
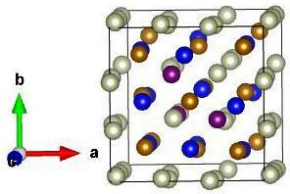
Supplementary material
Influence of structural disorder on magnetic order in FeRhCr alloys

Table S1. Models of supercells using to represent different Cr concentration in FeRhCr alloy for both spin configurations (FM and AFM). Color reference: Rh atoms are in gray, Cr atoms are in purple and Fe atoms are in gold (spin up ↑) and blue (spin down ↓). The corresponding volume of the crystal lattice (Vol cell) and energy per atom in cell (E/at) are included. The most stable energy values for the different Cr concentrations are highlighted in bold.

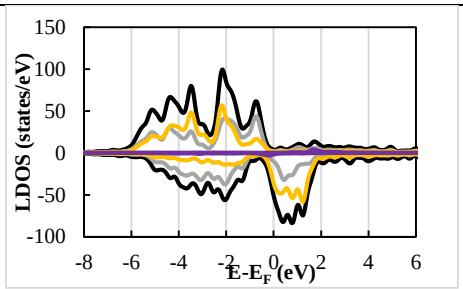
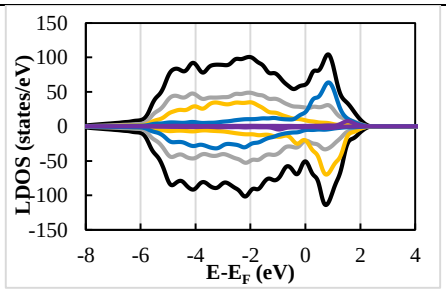
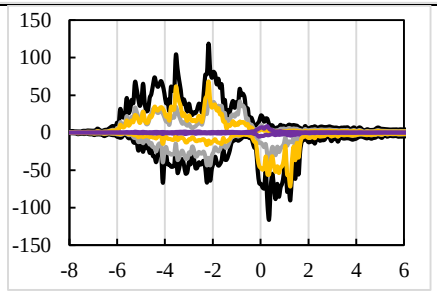
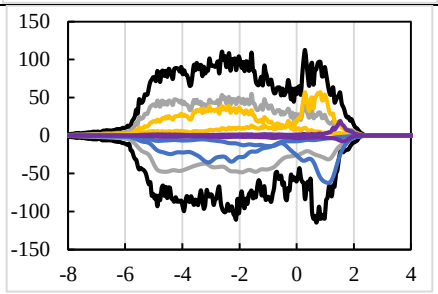
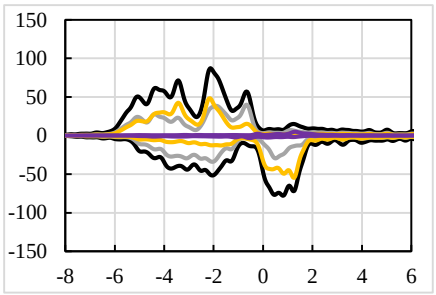
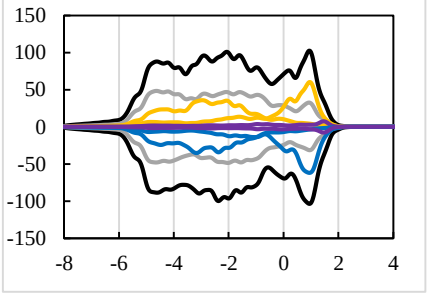
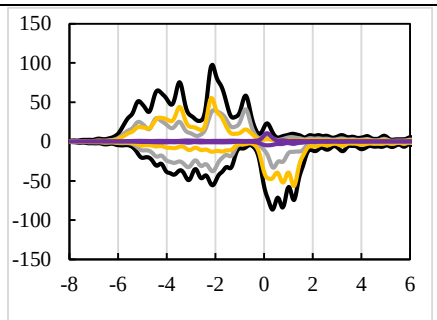
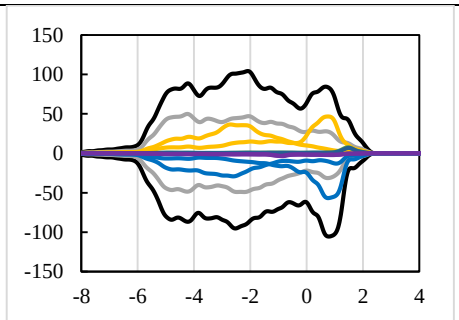
composition	FM	Vol cell (Å^3)	E/at (eV/at)	AFM	Vol cell (Å^3)	E/at (eV/at)
$Fe_{50}Rh_{50}$		732.5	**-7.789**		722.7	**-7.757**
$Fe_{50}Rh_{50}$		732.5	**-7.789**		707.3	**-7.789**
$Fe_{48.1}Rh_{50}Cr_{1.9}$ @1Fe (↑)		730.7	-7.793		723.9	-7.777
$Fe_{48.1}Rh_{50}Cr_{1.9}$ @1Fe (↓)		730.7	**-7.793**		709.5	**-7.807**
$Fe_{43.3}Rh_{50}Cr_{3.7}$		729.7	-7.799		708.1	-7.831
$Fe_{43.3}Rh_{50}Cr_{3.7}$		728.0	**-7.819**		706.0	**-7.835**
$Fe_{43.3}Rh_{50}Cr_{3.7}$		728.2	-7.798		701.8	-7.832

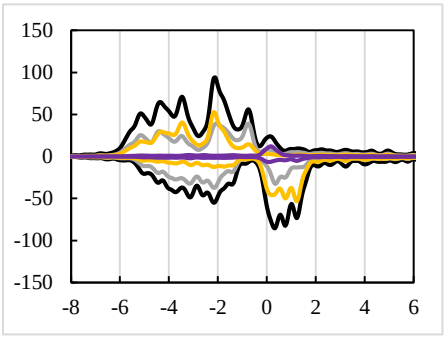
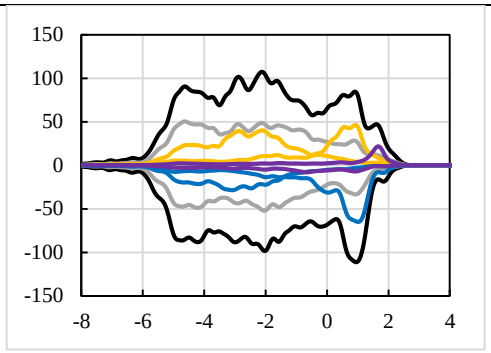
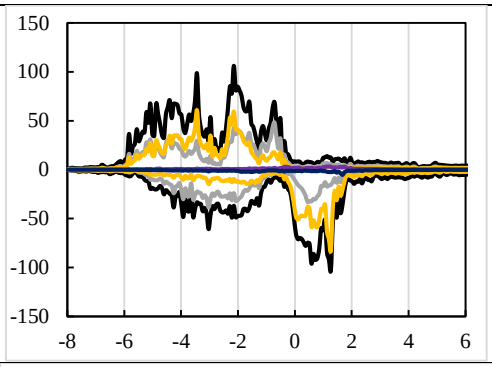
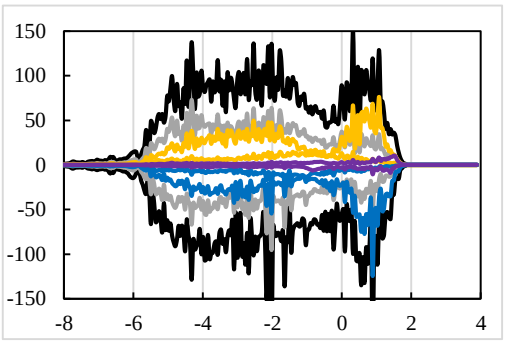
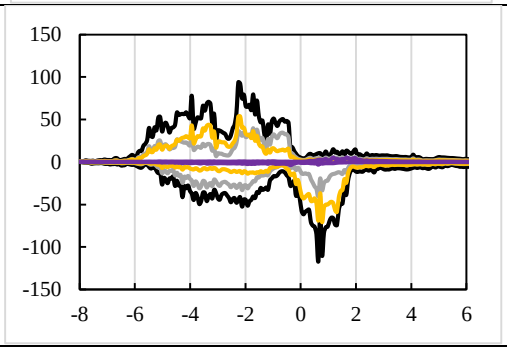
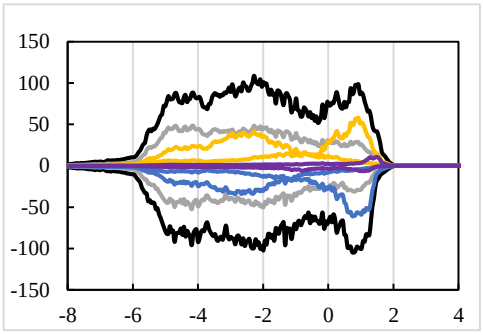
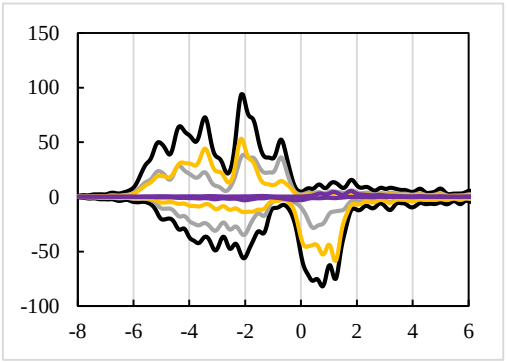
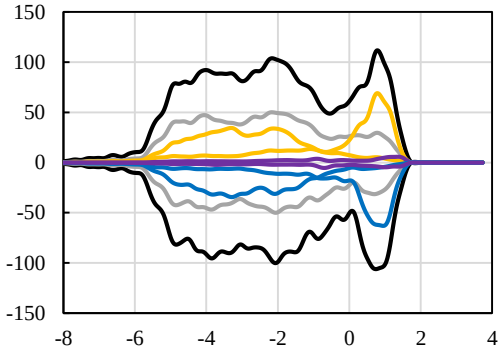
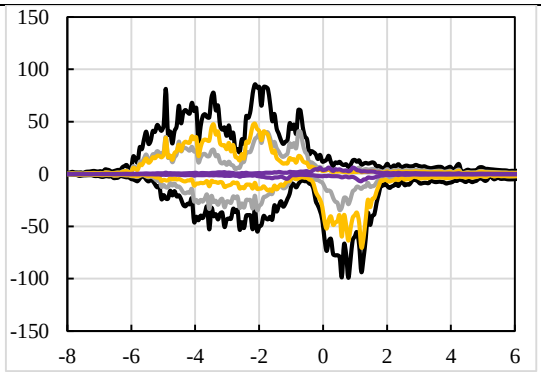
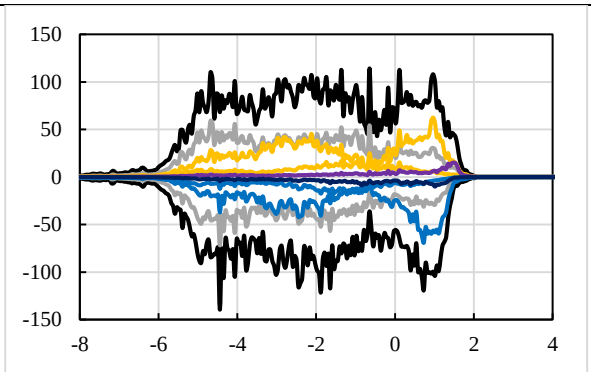
$Fe_{44.4}Rh_{50}Cr_{5.6}$		727.3	**-7.806**		705.2	**-7.855**
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		727.1	-7.832		706.4	-7.821
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		728.6	**-7.841**		699.7	**-7.842**
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		728.7	-7.838		709.8	-7.828
$Fe_{48.1}Rh_{46.3}Cr_{5.6}$		722.5	**-7.854**		696.3	**-7.863**
$Fe_{50}Rh_{48.1}Cr_{1.9}$		729.3	**-7.815**		703.6	**-7.785**
$Fe_{50}Rh_{46.3}Cr_{3.7}$		726.0	**-7.845**		692.8	**-7.849**
$Fe_{50}Rh_{46.3}Cr_{3.7}$		727.1	-7.842		716.3	-7.836
$Fe_{50}Rh_{46.3}Cr_{3.7}$		727.1	-7.842		704.5	-7.836

$Fe_{50}Rh_{44.4}Cr_{5.6}$		722.8	**-7.874**		696.8	**-7.856**

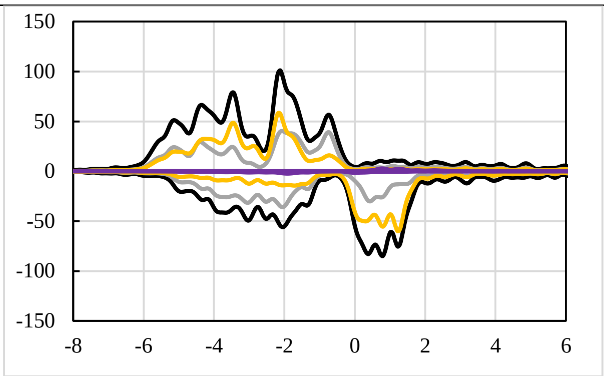
Reference color composition. Red: equiatomic - gold: @Fe doped - blue: @Fe and @Rh doped - black: @Rh doped

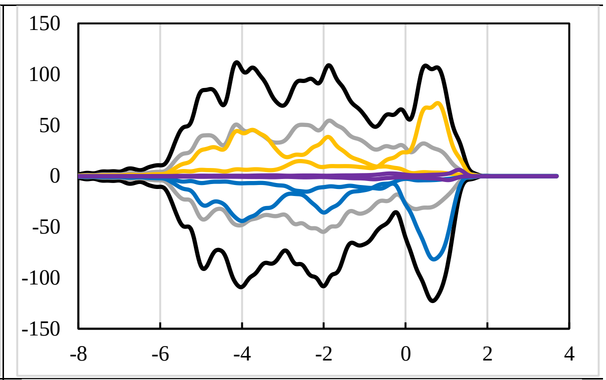
Table S2. (Color online) Local density of states (LDOS) of FeRh alloy at different contents of Cr obtained from FM and AFM magnetic configurations. The origin of the energy scale corresponds to the Fermi level. The spin-down (minority) were plotted as negative values to facilitate the visualization. Color reference: total DOS in black, LDOS of Fe (3*d*) in orange, Rh (4*d*) in gray and Cr (3*d*) in violet.

composition	**FM**	**AFM**
$Fe_{48.1}Rh_{50}Cr_{1.9}$ @1Fe (↓) or @1Fe (↑)		
$Fe_{43.3}Rh_{50}Cr_{3.7}$		
$Fe_{43.3}Rh_{50}Cr_{3.7}$		
$Fe_{43.3}Rh_{50}Cr_{3.7}$		

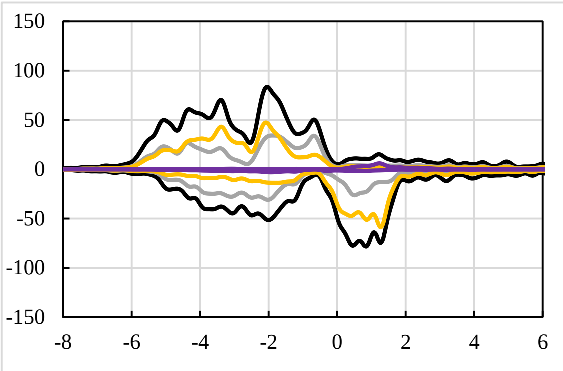
$Fe_{44.4}Rh_{50}Cr_{5.6}$		
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		
$Fe_{48.1}Rh_{48.1}Cr_{3.7}$		
$Fe_{48.1}Rh_{46.3}Cr_{5.6}$		

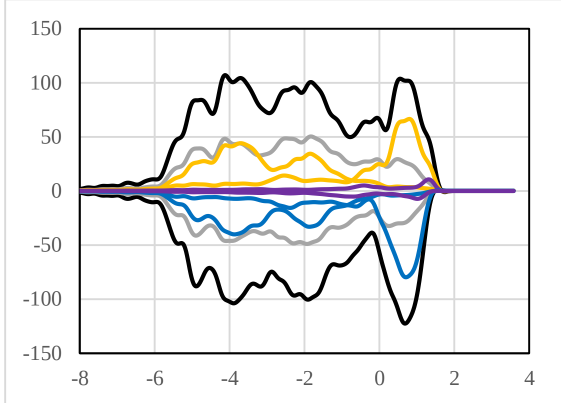
$Fe_{50}Rh_{48.1}Cr_{1.9}$



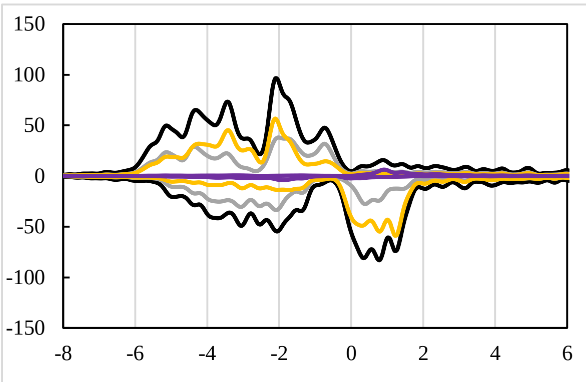


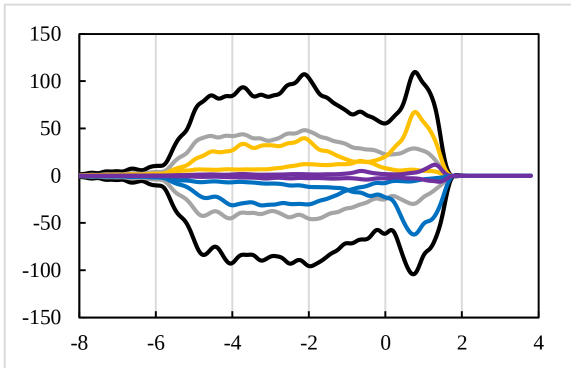
$Fe_{50}Rh_{46.3}Cr_{3.7}$



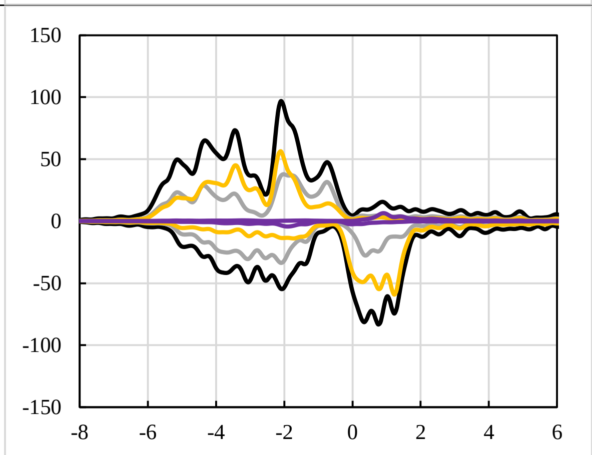


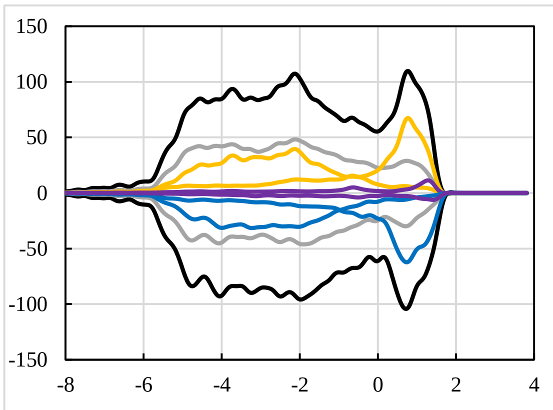
$Fe_{50}Rh_{46.3}Cr_{3.7}$





$Fe_{50}Rh_{46.3}Cr_{3.7}$





$Fe_{50}Rh_{44.4}Cr_{5.6}$