Effects of oxidation and chlorine defects on ferromagnetic $CrCl_3$ monolayer

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Layered vdW transition metals trihalides

Overview of the layered vdW transition metals trihalides MX_3 crystals

MCl_3

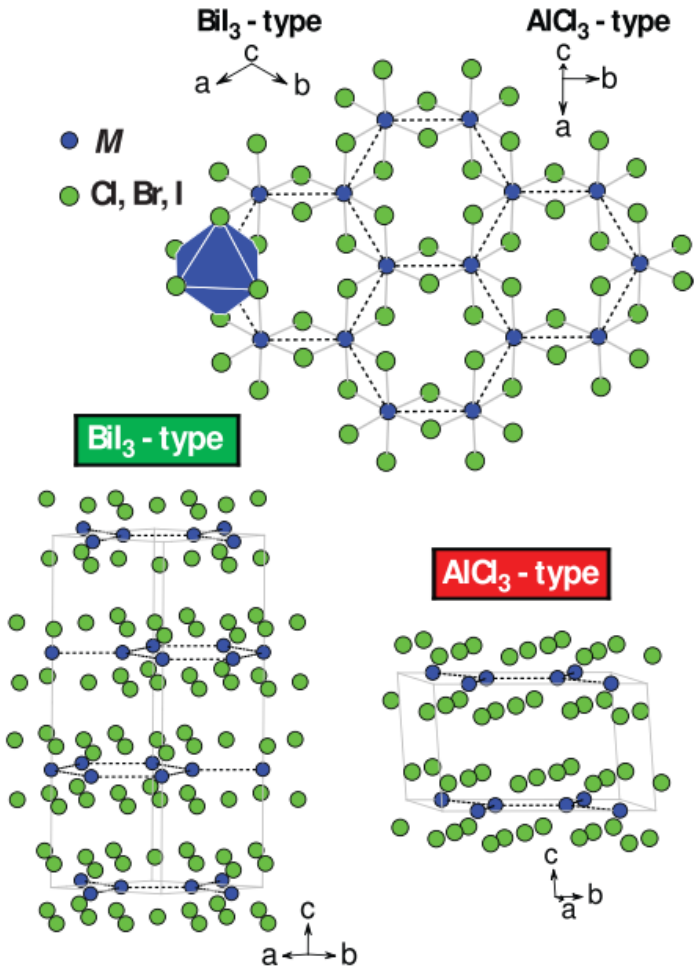
Ti	V	Cr	Mn	Fe	Co	Ni
Zr	Nb	Mo	Tc	Ru	Rh	Pd
Hf	Ta	W	Re	Os	Ir	Pt

MBr_3

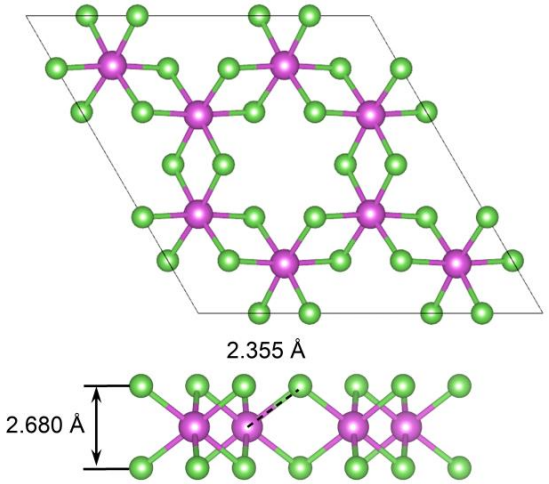
Ti	V	Cr	Mn	Fe	Co	Ni
Zr	Nb	Mo	Tc	Ru	Rh	Pd
Hf	Ta	W	Re	Os	Ir	Pt

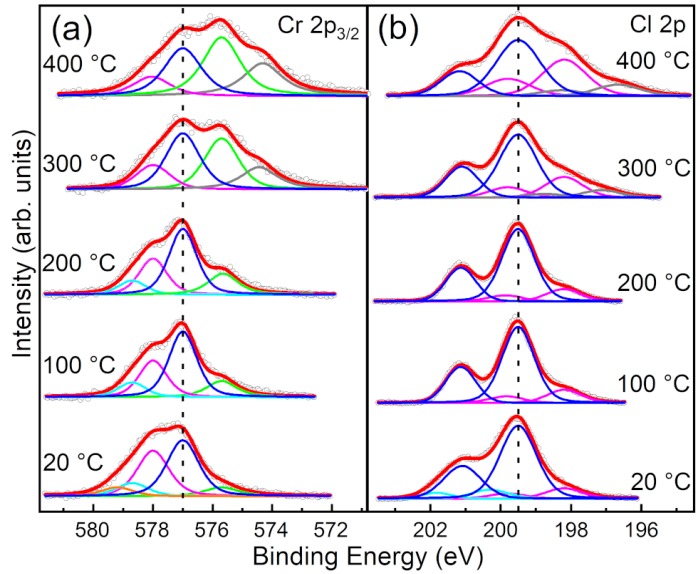
MI_3

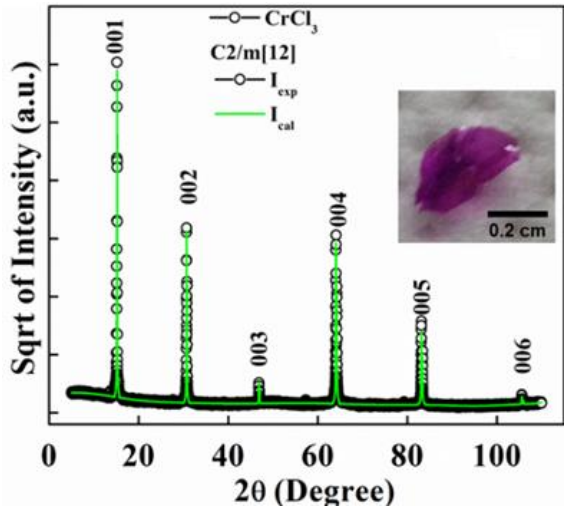
Ti	V	Cr	Mn	Fe	Co	Ni
Zr	Nb	Mo	Tc	Ru	Rh	Pd
Hf	Ta	W	Re	Os	Ir	Pt

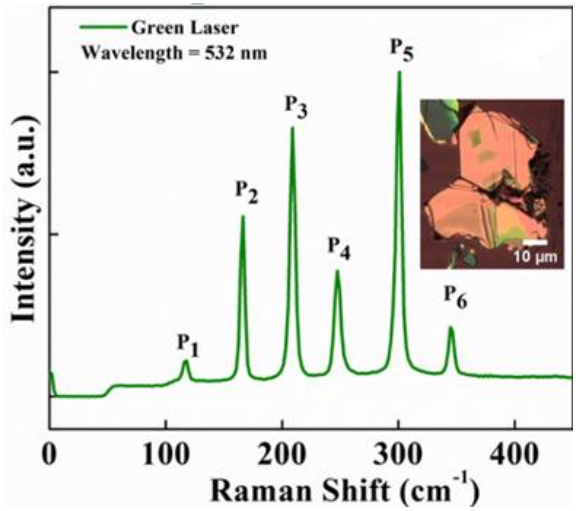


$CrCl_3$ crystals





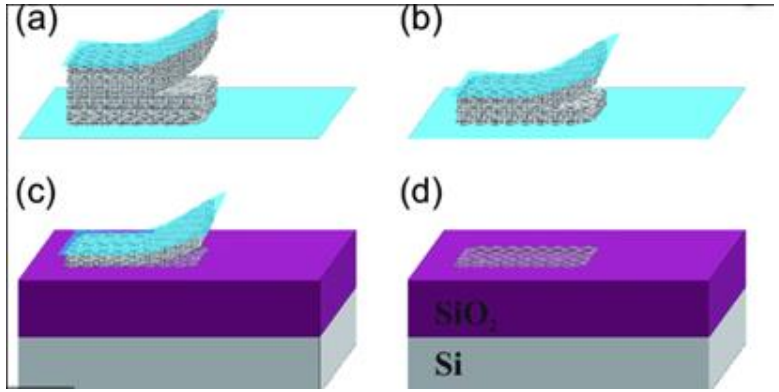


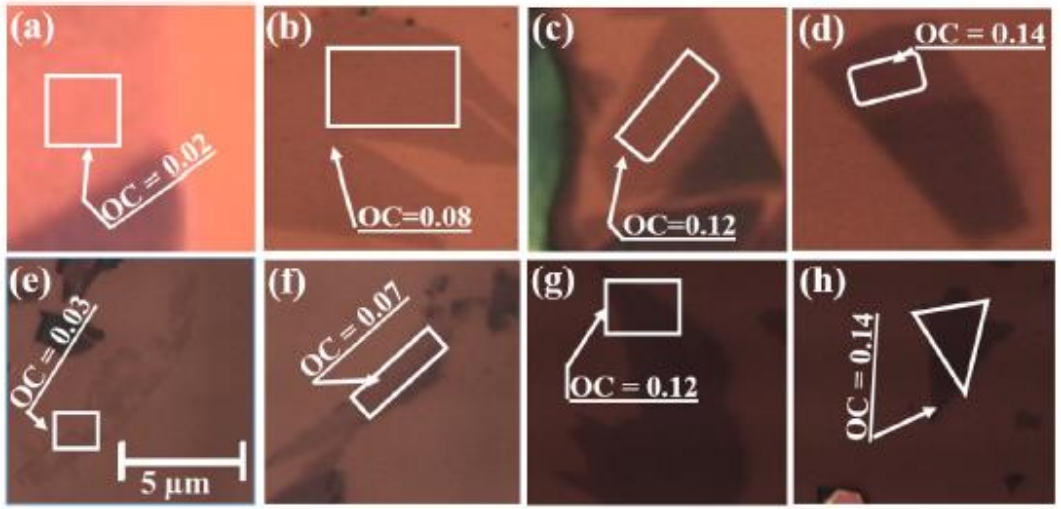


M. McGuire et al., Crystals, 7, 121 (2017)
Kazim S. et al. Nanotechnology, 31, 395706 (2020)
D. Mastrippolito et al., Nanoscale Advances, 3, 4756-4766 (2021)

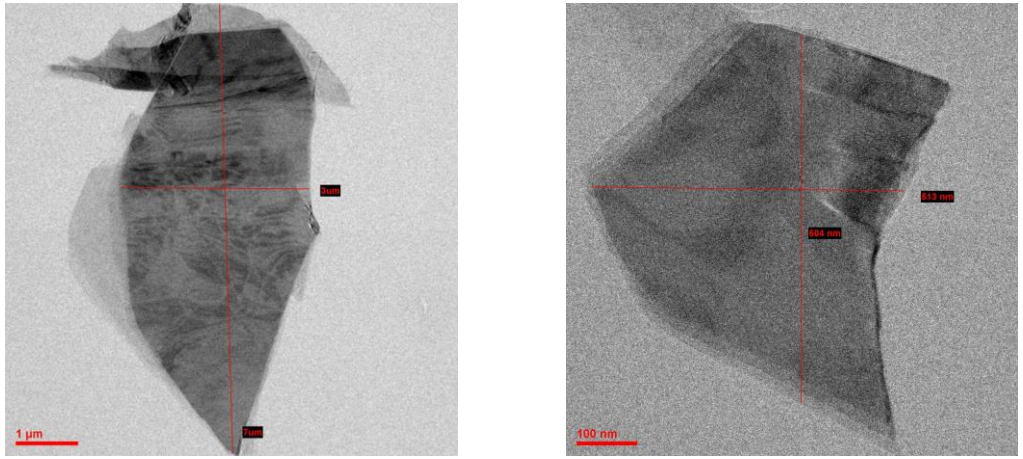
$CrCl_3$ nanoflakes

Blue tape mechanical exfoliation and atomic layer deposition

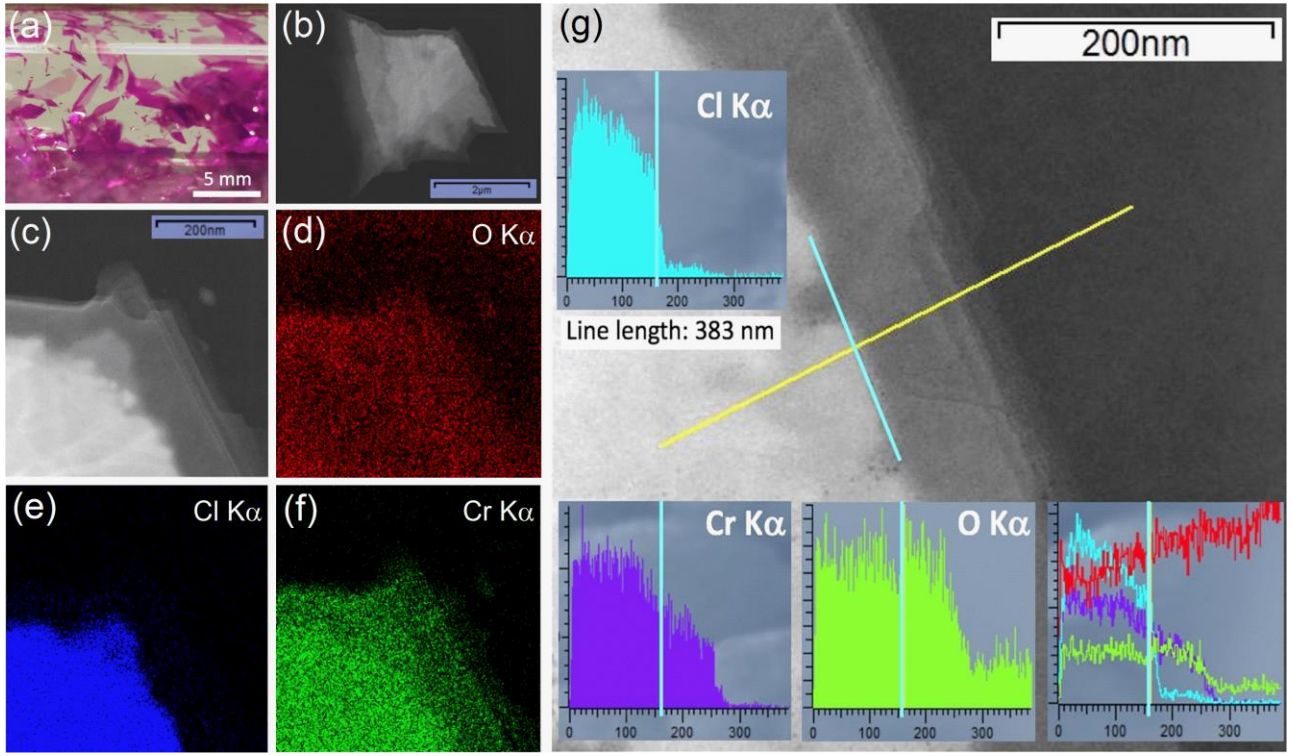




Optical images on a 270 nm SiO_2/Si substrate (a-d) and (e-h) on a 285 nm SiO_2/Si substrate (e-h)



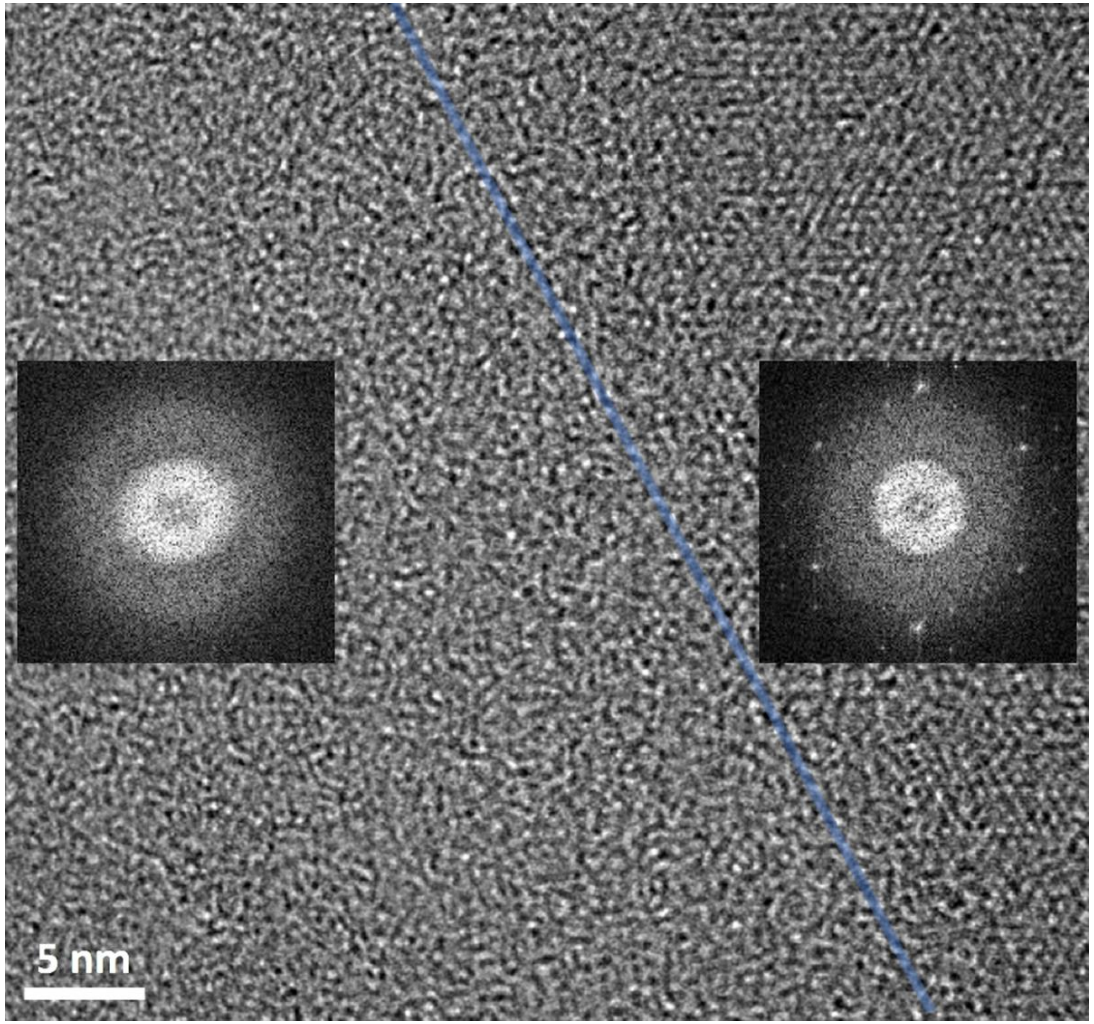
TEM images of freshly exfoliated $CrCl_3$



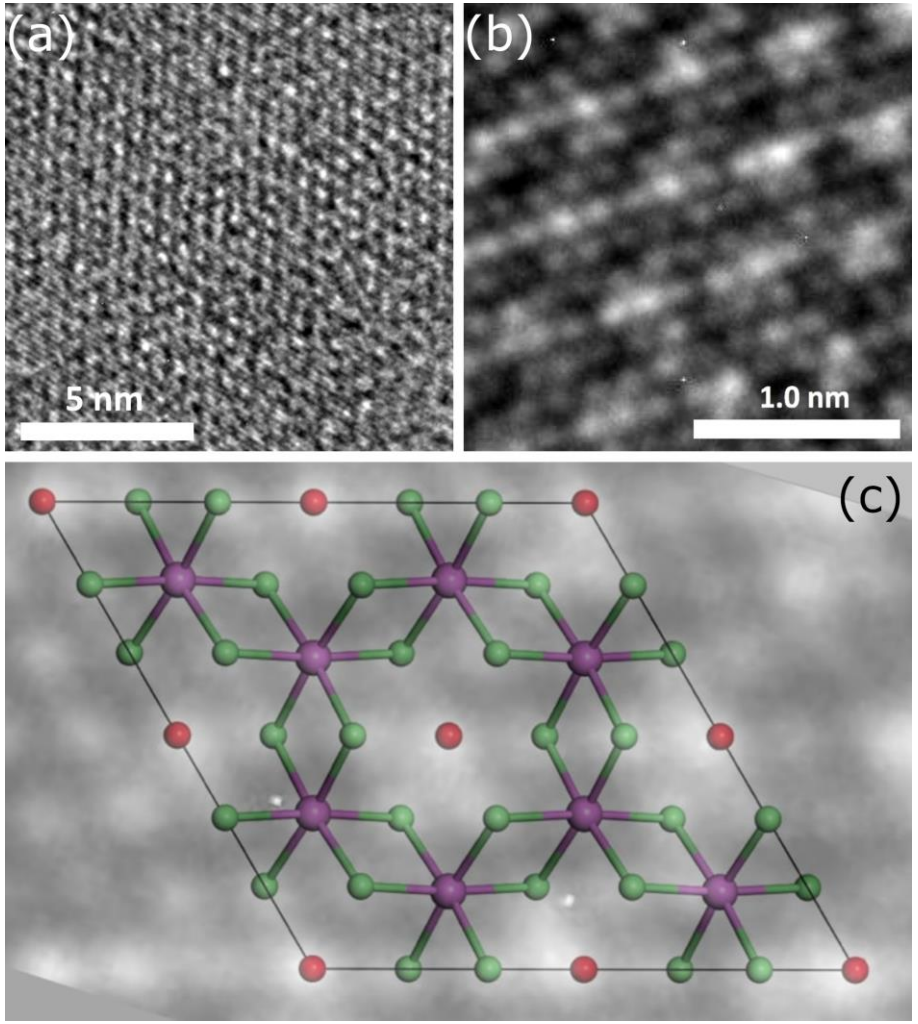
EDX micro-analysis

Kazim S. et al. Nanotechnology, 31, 395706 (2020)
D. Mastrippolito et al., Nanoscale Advances, 3, 4756-4766 (2021)

$CrCl_3$ nanoflakes



Coexistence of amorphus and ordered $CrCl_3$ phases



Ordered O-$CrCl_3$ structure

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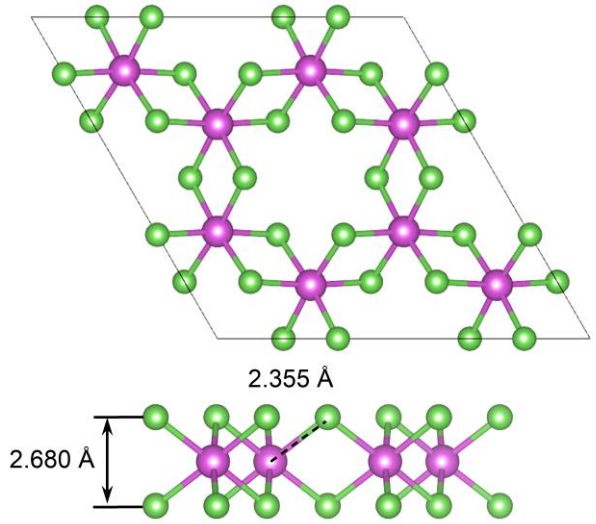
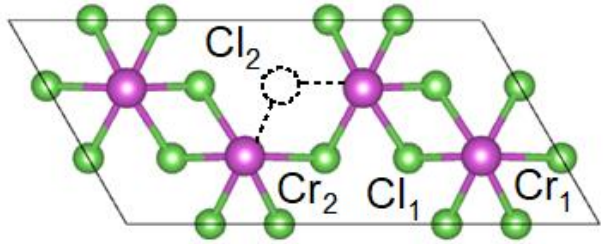
Monolayer $CrCl_3$ phases

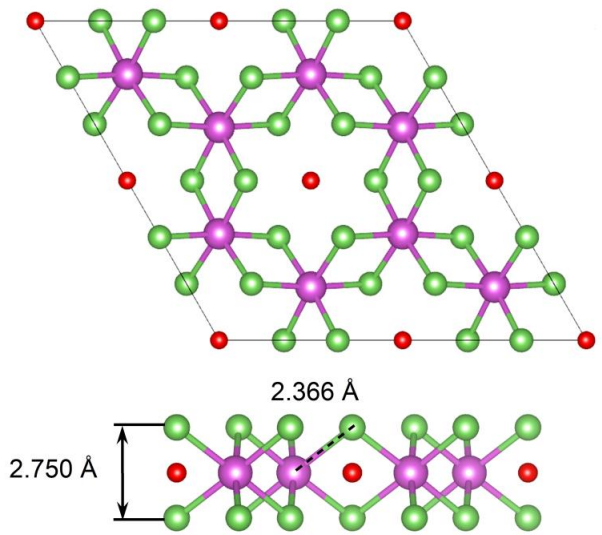
Pristine $CrCl_3$

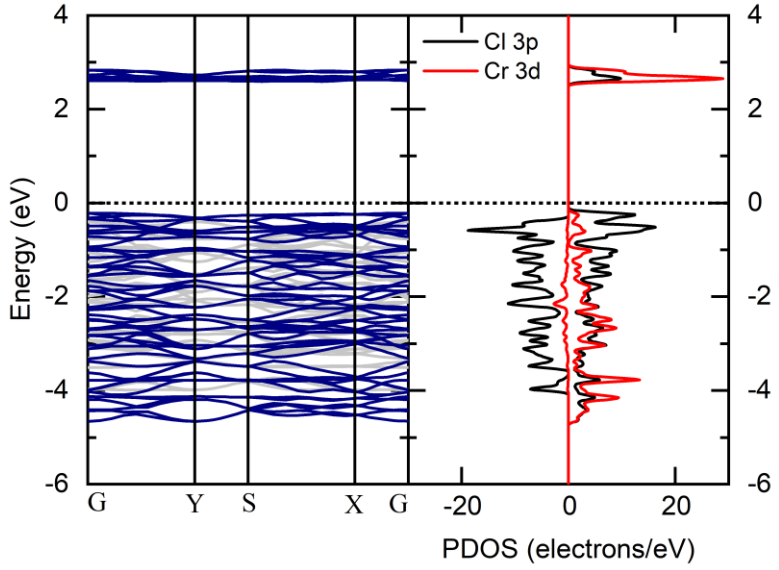


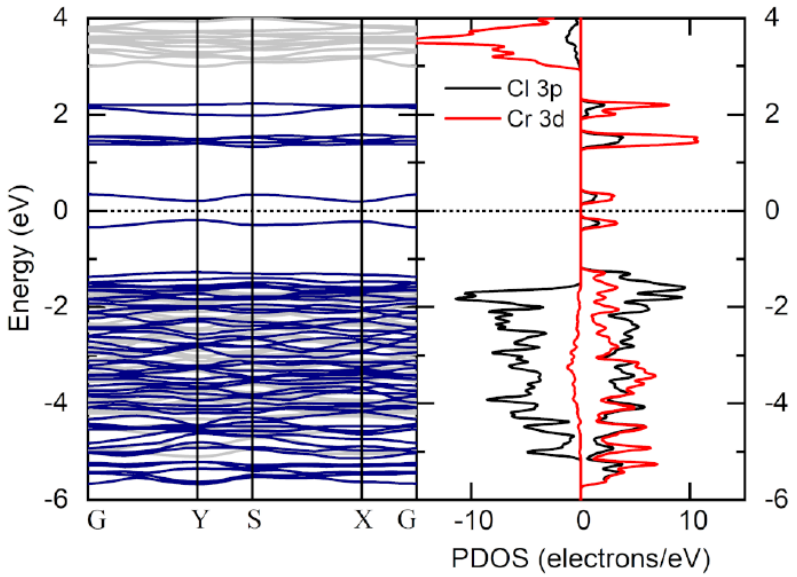
Cl-defective 2X1 supercell ($CrCl_{2.75}$)

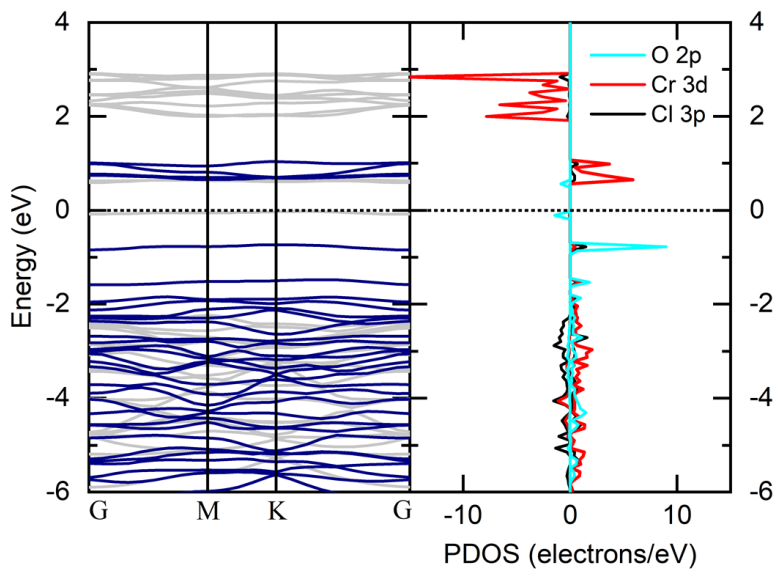


Ordered O-$CrCl_3$









Spin-resolved Electronic Bands

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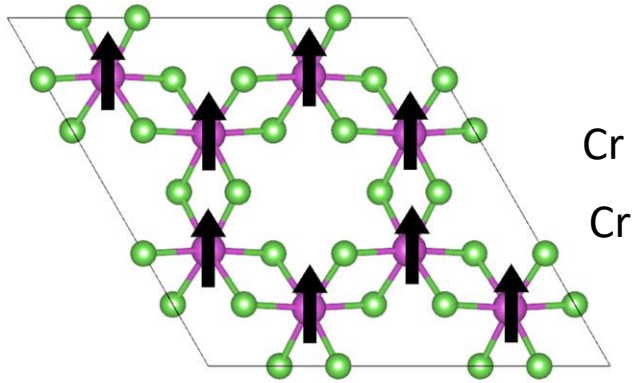
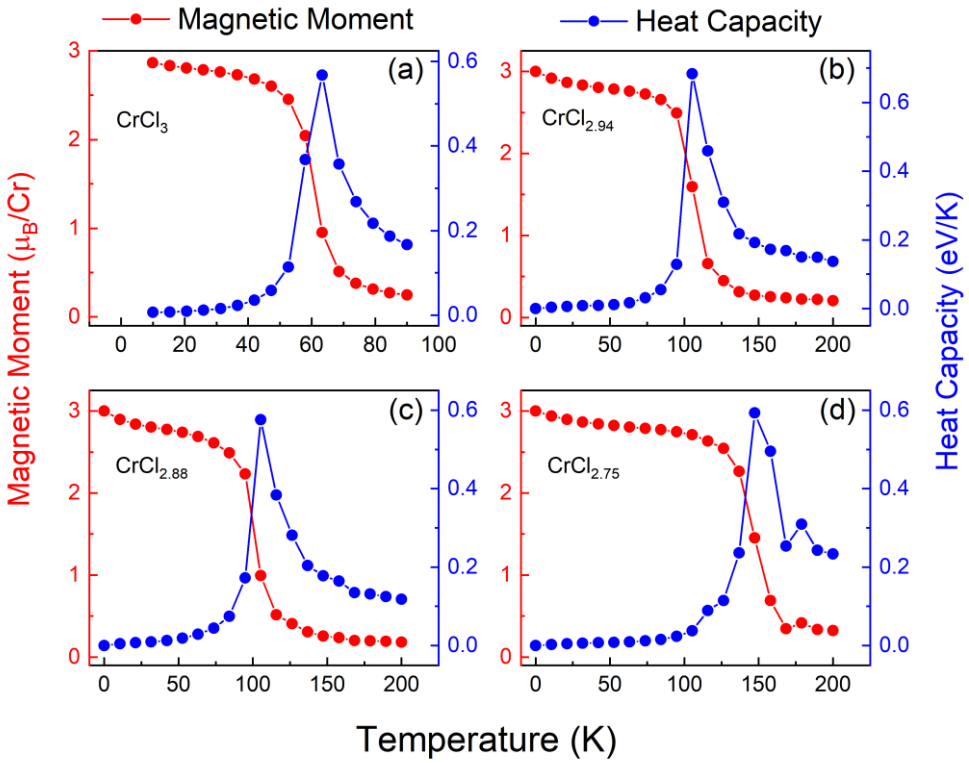
Magnetic properties of Cl-defective $CrCl_3$



Ferromagnetic $CrCl_3$

Cr magnetic moment (3.15 μ_B) of $CrCl_3$

Cr magnetic moment (3.53 μ_B) of $CrCl_{2.75}$



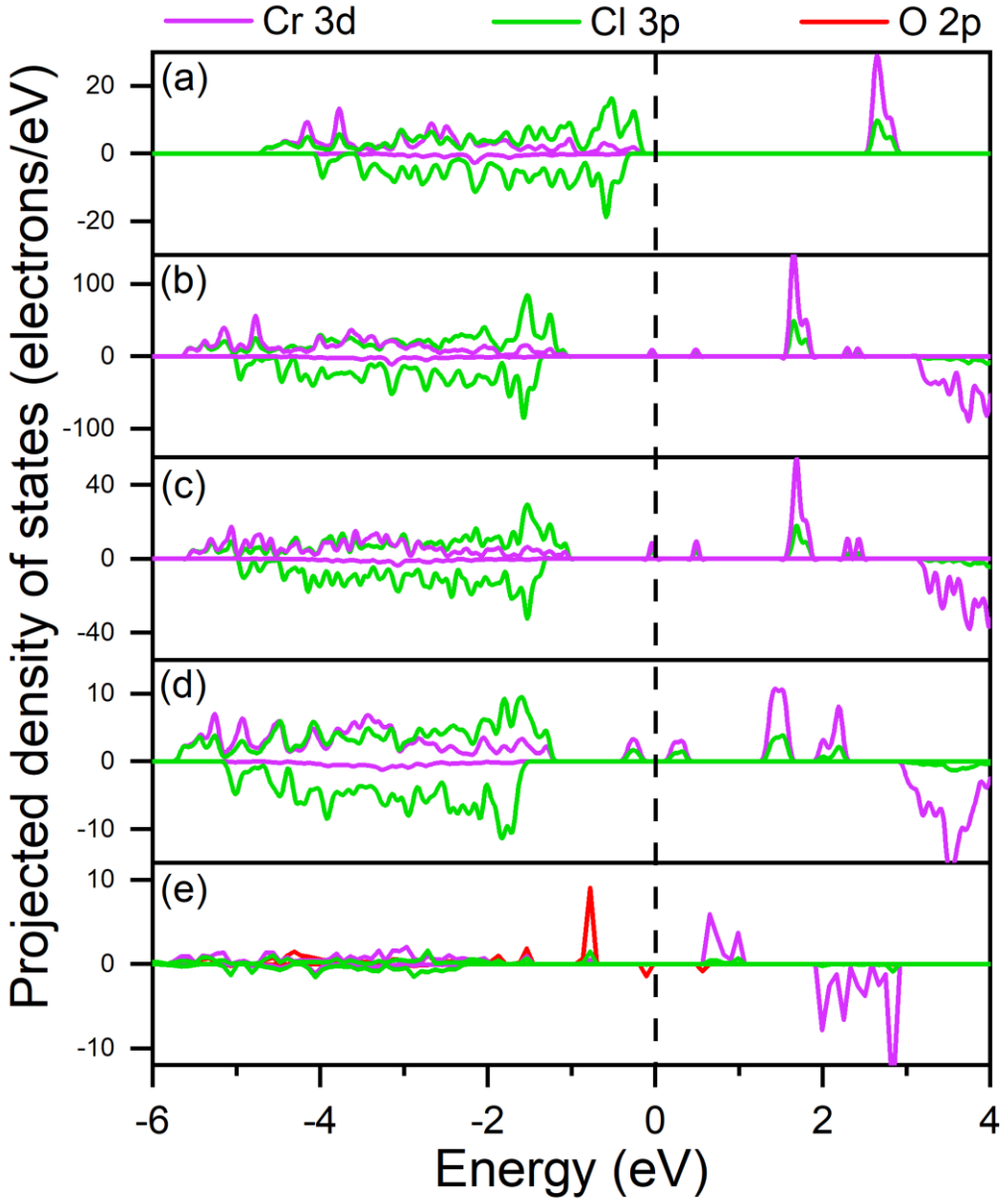
a) Monolayer $CrCl_3$

b) Monolayer $CrCl_{2.94}$

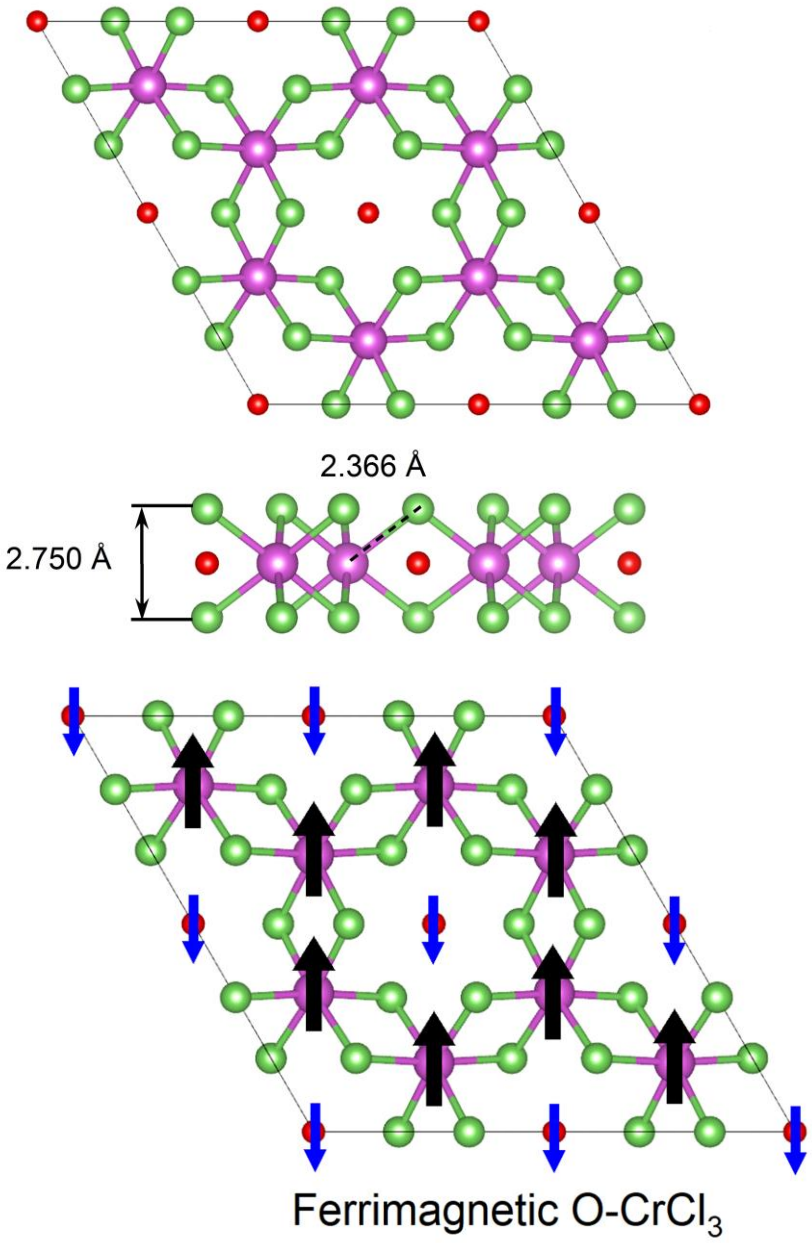
c) Monolayer $CrCl_{2.88}$

d) Monolayer $CrCl_{2.75}$

e) Monolayer O-$CrCl_3$



Magnetic properties of O-$CrCl_3$

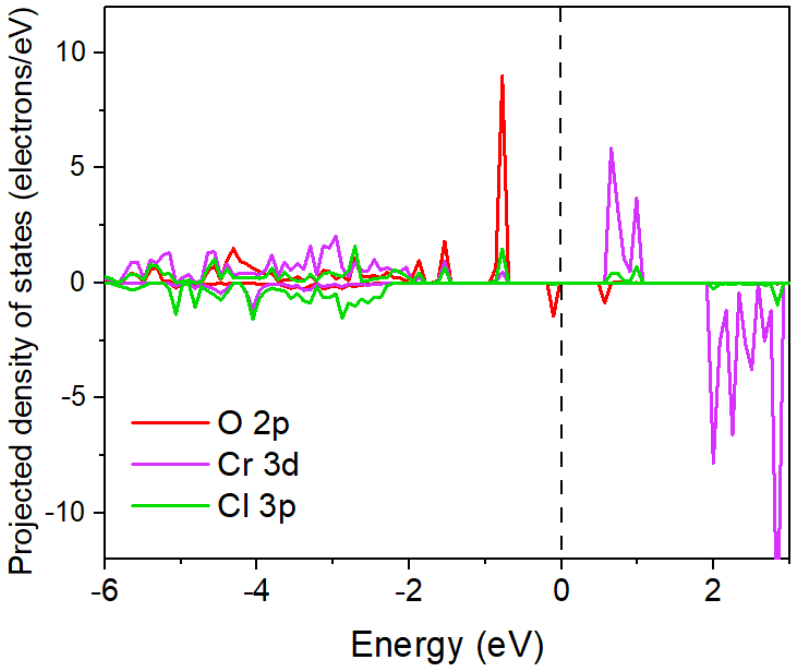


Cr magnetic moment (3.05 μ_B) of O-$CrCl_3$

O magnetic moment (1.37 μ_B) of O-$CrCl_3$

Magnetic moment (4.27 μ_B) per unit cell (Cr_2Cl_6O)

Mean field T_C (110 K)



Conclusions

- Cl-vacancy defective and ordered oxidized induced extrinsic phases in 2D $CrCl_3$
- Halogen vacancies represent a low-cost method to enhance the magnetic ordering temperature of the 2D transition metal trihalides class
- Oxygen intercalated impurities result in unconventional 2D ferrimagnetic hexagonal system

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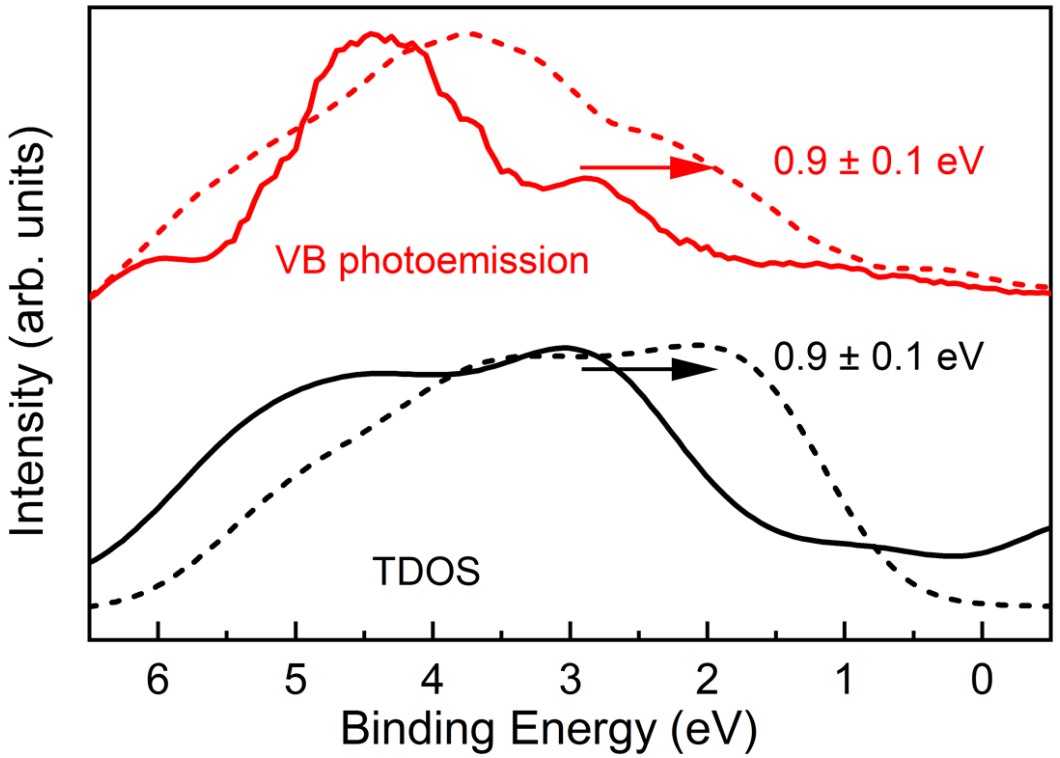
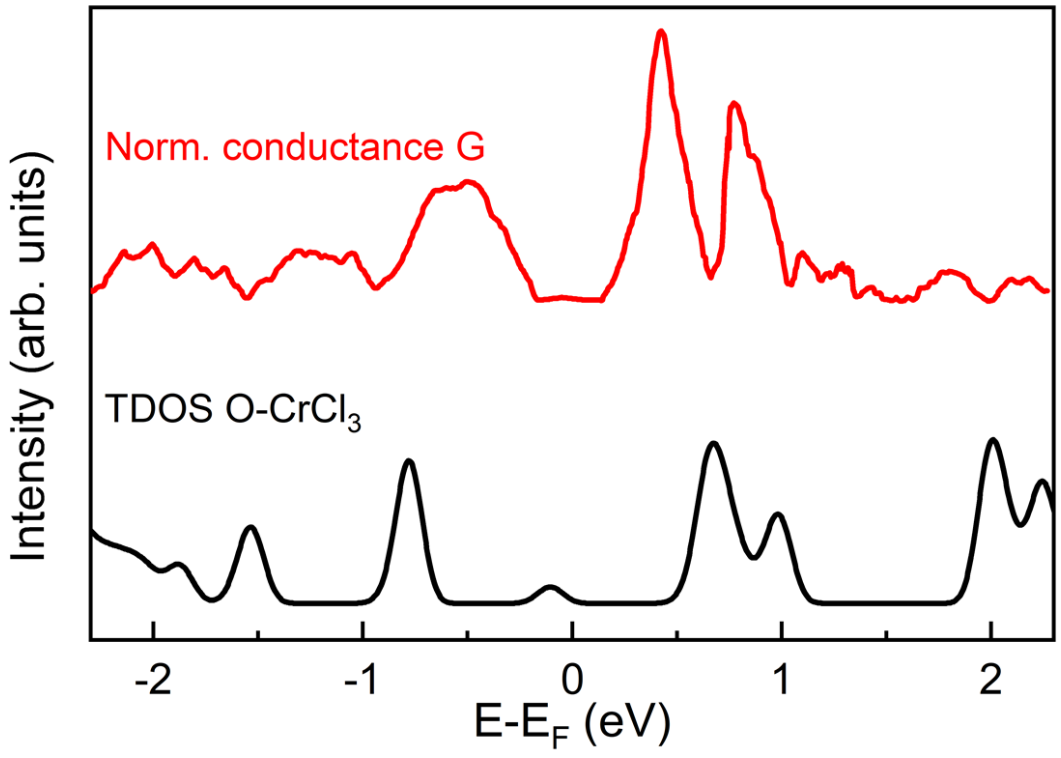
Thank you for the attention

Valence and conduction bands



Surface-sensitive UPS (red curve) and bulk-sensitive XPS (dashed red curve) valence bands compared with TDOS of O–$CrCl_3$ (black curve) and the 1.85% Cl-defective $CrCl_3$ (dashed black curve) structure.



TDOS of O–$CrCl_3$ (black) compared with surface normalized conductance (red)

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