

Electronic Supporting Information (ESI) for:

High-Pressure Magnetic Properties and Electrical Transport Behaviors of Half-Metallic Ferromagnet CrO₂

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Table S1. Details of the refinement for X-ray diffraction pattern.

Pressure	Ambient pressure
cryst syst	Tetragonal
space group	$P4_2/mnm$
Refine mode	Le Bail fit
a/Å	4.41492
b/Å	4.41492
c/Å	2.91466
volume/Å ³	56.811
R-factors	R _p =0.00300 R _{wp} =0.00585 R _{exp} =0.0217 Chi2=0.0706
radiation	Cu Kα ($\lambda_{K\alpha 1}$ =1.54059 Å, $\lambda_{K\alpha 2}$ = 1.54431 Å)
2θ range	20-90°
step	0.02

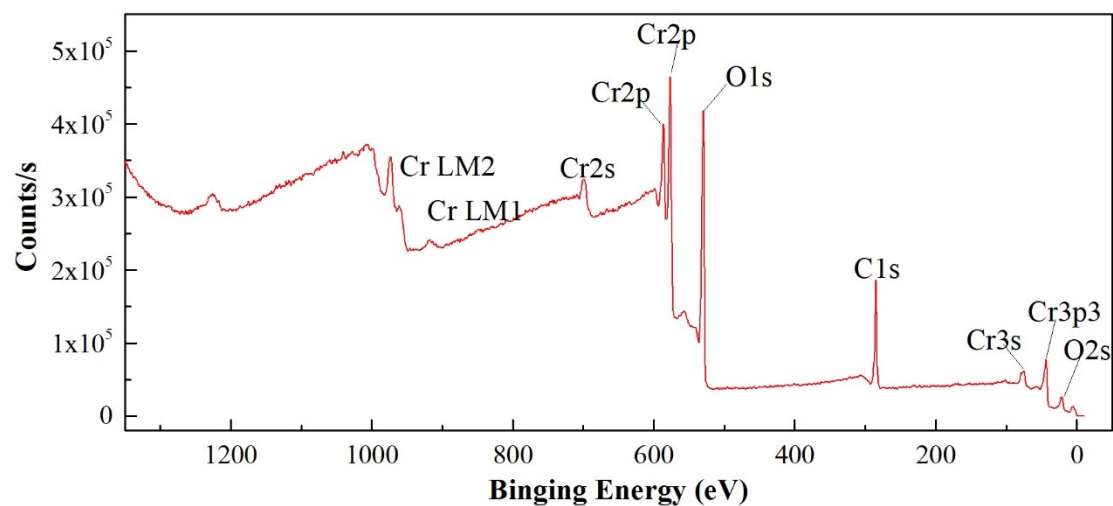


Fig. S1 X-ray Photoelectron Spectroscopy of CrO_2 at ambient conditions, C element is used for instrument calibration.

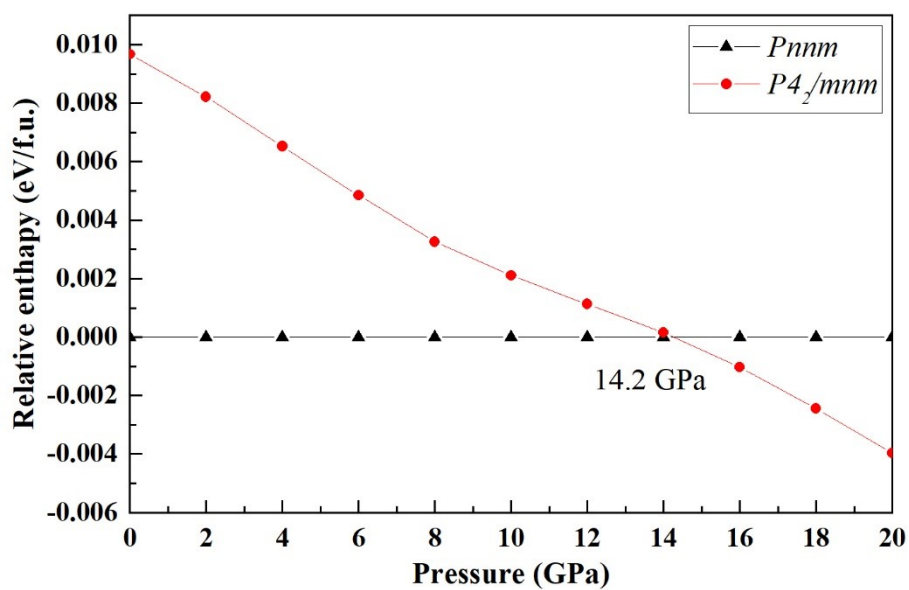


Fig. S2 Relative enthalpies of CaCl_2 -type ($Pn\bar{m}$) structure of CrO_2 compared to the rutile-type ($P4_2/mnm$) structure under different pressures.

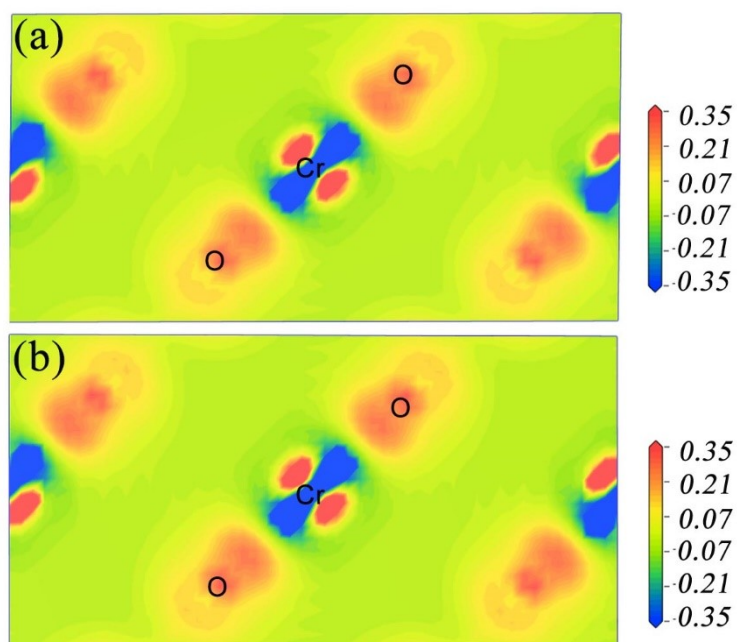


Fig. S3 The calculated difference charge density of the rutile-type structure (10 GPa) and the CaCl₂-type structure (16 GPa) for CrO₂.