Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

A facile synthesis of phase-pure $FeCr_2Se_4$ and $FeCr_2S_4$ nanocrystals via wet chemistry method

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<u>Conductivity mechanism:</u>

A simplified expression of conductivity can be obtained by converting the previous equation. As shown in Debye's isotropic continuum model,[1-3] the resulting expression is:

$$I = H^2 Q_d^5 / 6\pi^2 K_b T^2 \sum_{s}^{4} (C_s^4) \int_0^1 dx\, x4\, \Gamma \bar{n}(\bar{n}+1) \qquad (1)$$

$\bar{n}$In equation (1), where $x = Q/Q_d$ and $\Gamma$and understood as functions of x, T and polarization s. The total relaxation is $\Gamma_{qs}^{-1} = \sum \Gamma_{qs}^{-1}(i)$, with $\Gamma_{qs}^{-1}(i)$ being the relaxation due to the phonon mechanism. The conductivity can be approximate as:

$$I = (H^2/3N_0 \Omega K_B T^2) \sum_{qs}^{0} \sigma Cs^2(q) \omega^2(qs) \tau(qs) nqs(nqs+1) \qquad (2)$$

$$\sigma = \lambda_L / L * T \qquad (3\text{-}1)$$

$$\Delta\Omega = \Delta W * V * L_s^{1/2} / W * V = \Delta W * L_s^{1/2} / W \qquad (3\text{-}2)$$

In equation (2), provided reasonable forms of the phonon-dispersion relation $\omega = \omega(\mathbf{q}s)$ and relaxation time $\tau(\mathbf{q}s)$ are chosen, it should be straightforward to be proved by the conductivity of a crystal lattice contribution (λ_L). The nature of conductivity is dependent on the NCs's λ_L, where L is the Lorenz factor, σ stands for the extent of NCs' crystallization; T is the temperature value in conductivity measurements (3-1). The related resistivity ΔΩ which is dependent on the NCs' size paremeter(L_s), where ΔW is the increase over the crystal resistivity W, L_s is the average grain size, V is the volume of NCs (3-2).

References:

[1] Sun, Y.; Rogers, J. A. Inorganic semiconductors for flexible electronic. *Adv Mater.* 2007, **19**, 1897.

[2] Watari, K.; Shinde, S. L. High thermal conductivity materials. *MRS Bulletin.* 2001, **26**, 440.

[3] Watari, K.; Hirao, K.; Toriyama, M.; Ishizaki, K. Effect of grain size on the thermal conductivity of Si_3N_4. *J. Am. Ceram. Soc.* 1999, **82**, 777.

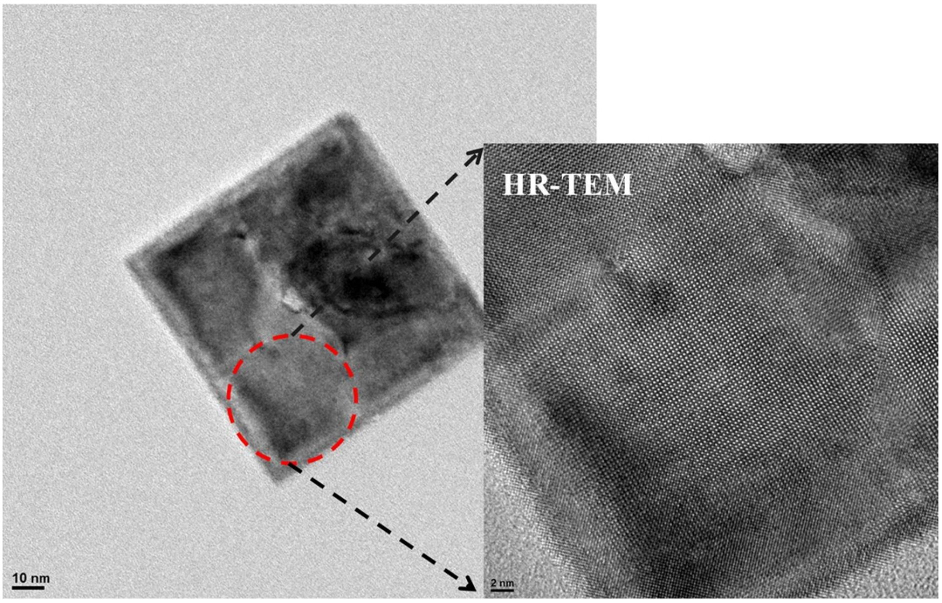


Figure S1: The TEM and HR-TEM images of single $FeCr_2Se_4$ NCs. Inserted scale bars are 10nm and 2nm, repescitively.

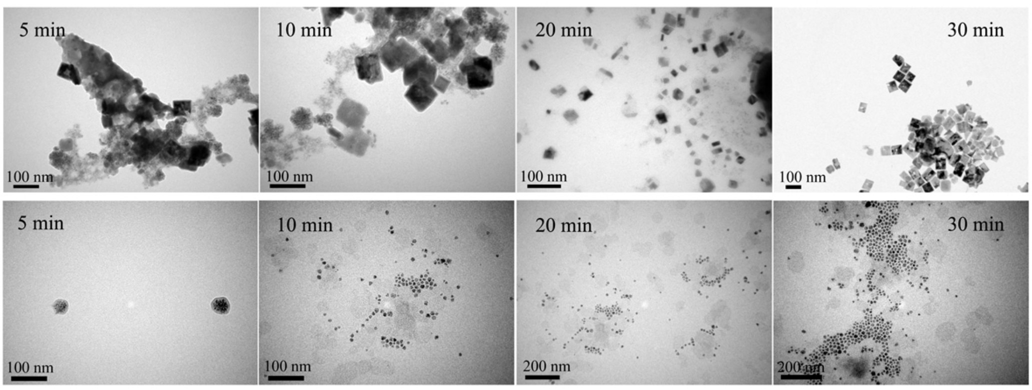
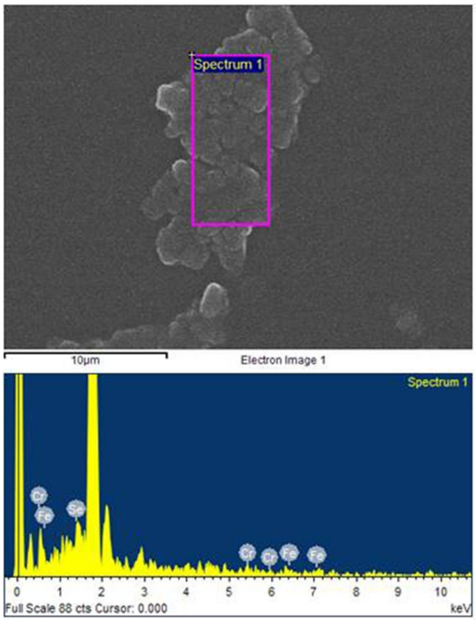
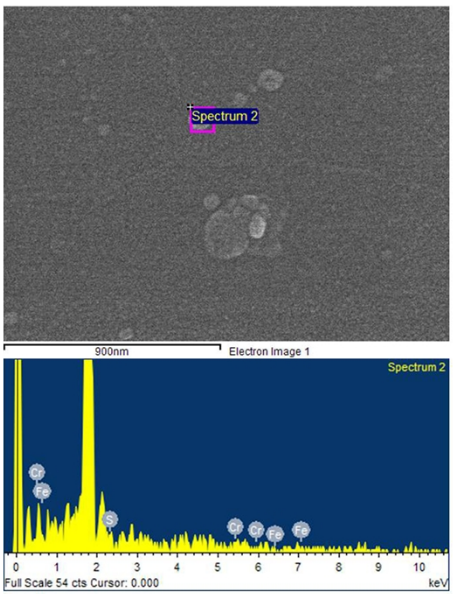


Figure S2: The TEM images of growth process: $FeCr_2Se_4$ (up) and $FeCr_2S_4$ (bottom).



Element	Weight%	Atomic%
Cr K	26.44	25.53
Fe K	13.36	16.34
Se L	60.20	58.13
Totals	100.00	

Figure S3: (a) FE-SEM image of OLA-capped NCs. (b) SEM-EDS spectra of $FeCr_2Se_4$ NCs.



8ij	Weight%	Atomic%
S K	53.22	51.67
Cr K	31.18	34.27
Fe K	14.59	14.06
Totals	100.00	

Figure S4: (a) FE-SEM image of OLA-capped NCs. (b) SEM-EDS spectra of $FeCr_2S_4$ NCs.

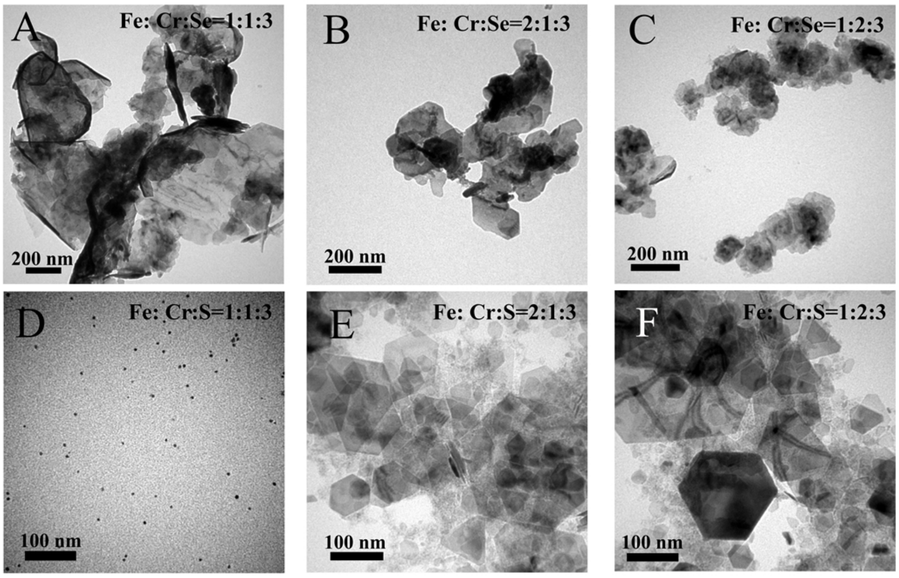


Figure S5. Representative TEM images of the products collected from the reaction with the same condition with different precursor molar ratio used in the synthesis of nanocrystals.

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The TGA data of $FeCr_2Se_4$ NCs (black) and $FeCr_2S_4$ NCs (red) were obtained (see Figure S6). For the $FeCr_2Se_4$ and $FeCr_2S_4$ NCs, the onset of decomposition occurred at 260 °C and 254 °C, and the decomposition temperature of $FeCr_2Se_4$ and $FeCr_2S_4$ NCs were 670 °C and 750 °C with a mass loss of 32.5% and 22.5%, respectively.

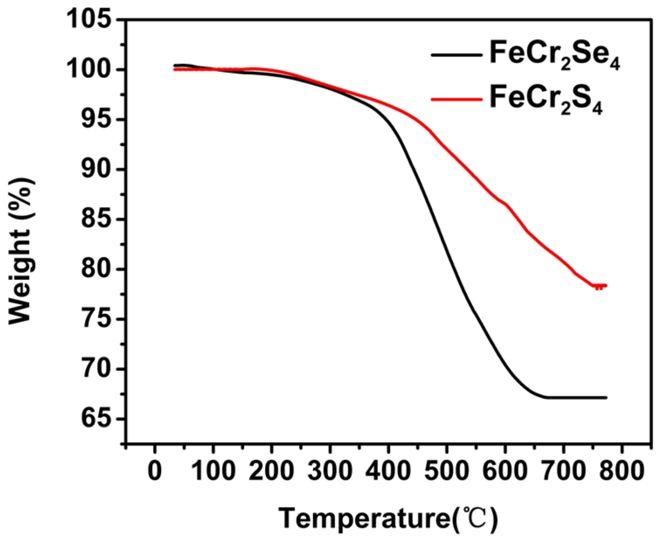

Figure S6: Thermal gravimetric analyses of $FeCr_2Se_4$ and $FeCr_2S_4$ NCs.

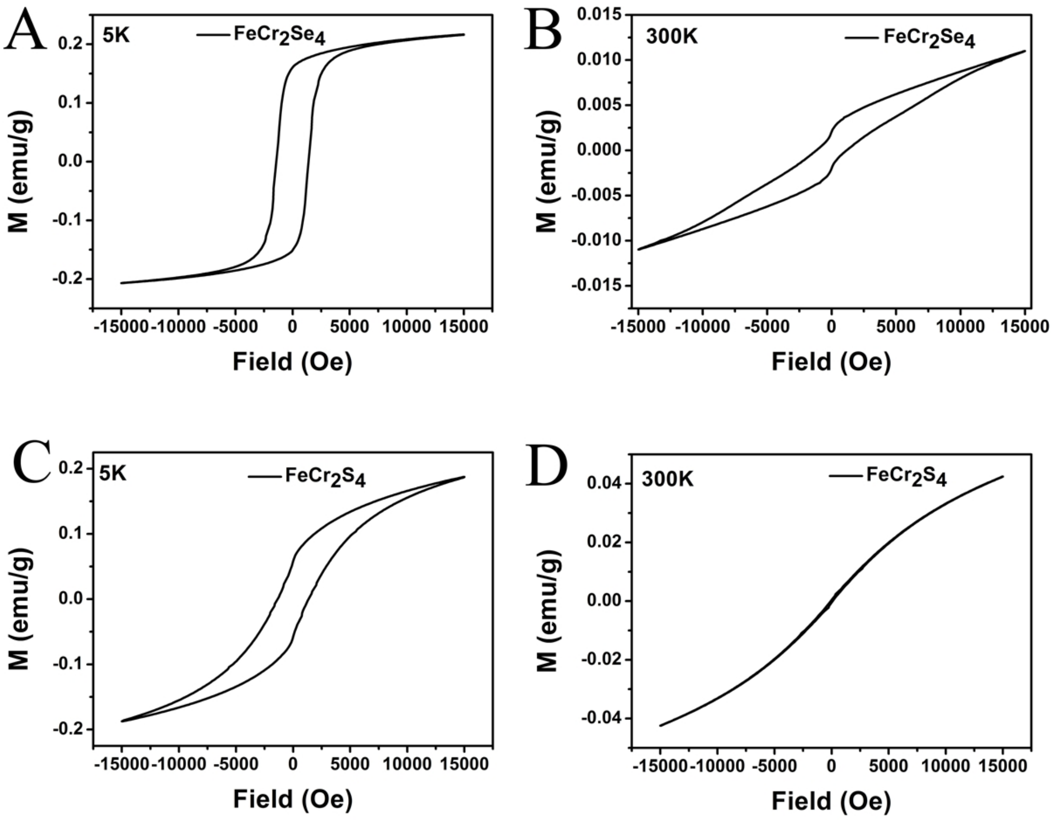

Figure S7 Magnetization (*M*) as a function of field (*H*) for $FeCr_2Se_4$ and $FeCr_2S_4$ NCs at (A, C) 5 K and (B, D) 300 K

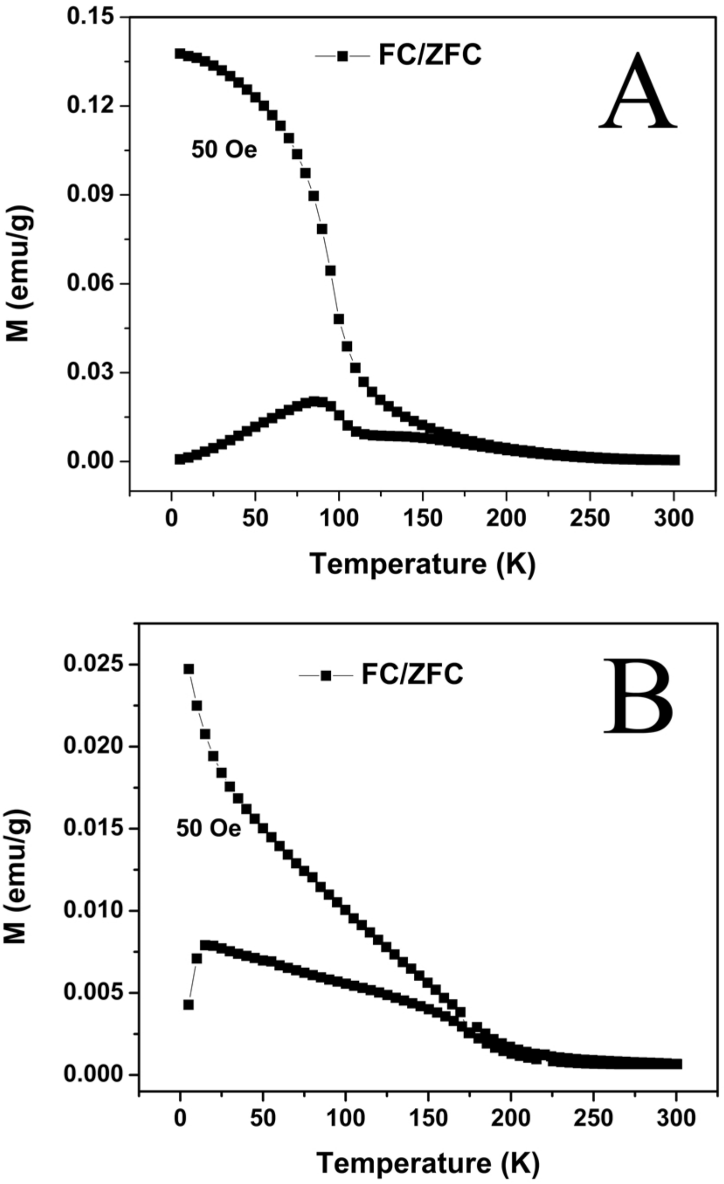

Figure S8: Magnetization (M) as a function of temperature for field-cooled (FC) and zero-field-cooled (ZFC) measurements at 50 Oe for $FeCr_2Se_4$ (A) and $FeCr_2S_4$ (B) respectively.

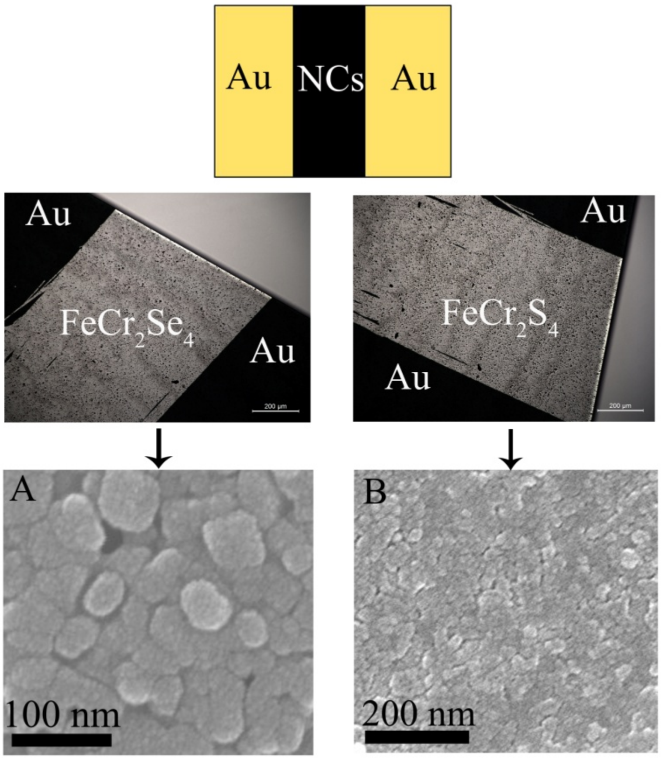

Figure S9: Simple fabrication schematic diagram(upper image) and two point Au electrode pad (insert scale bar is 200 micrometer); and SEM images of $FeCr_2Se_4$ film (A) and $FeCr_2S_4$ film (B), respectively.

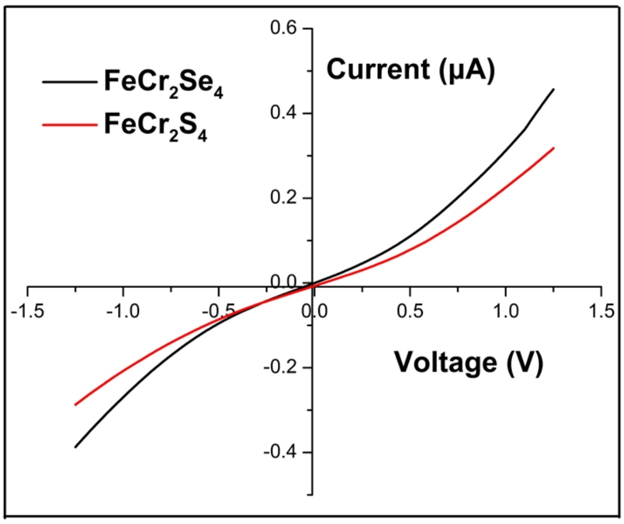

Figure S10: I-V curves of drop-casting films built from NCs, the range of voltage was from -1.25eV~1.25eV.