Supplementary Information

Effect of Cr-doping on the electronic structure and work function of α-Fe_2O_3 thin films

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1. The influences of U parameter
2. Different spin configurations of Cr-doped α-Fe_2O_3 thin films
3. The work function of the films

1. The influences of U parameter

We have examined the U and J values for Fe and Cr 3d orbitals for bulk α-Fe_2O_3 and α-Cr_2O_3 (1×1×1). Table S1 lists the calculated indirect band gap values and magnetic moments. The band gap increases with increasing U parameter for both α-Fe_2O_3 and α-Cr_2O_3. Comparing to the experimental data for energy gap of α-Fe_2O_3 (2.1-2.2 eV) [1,2] and α-Cr_2O_3 (3.4 eV or an optical band gap of 3.1 eV) [3,4], U = 6 eV provides a good description of the band gap for both α-Fe_2O_3 and α-Cr_2O_3. In our following calculations, we used U=6 eV and J=1 eV for both Fe and Cr 3d states.

Table S1. The calculated indirect band gap values and magnetic moments for bulk α-Fe_2O_3 and α-Cr_2O_3 (1×1×1). J is set to be 1 eV for Fe or Cr 3d orbitals.

U values	α-Fe_2O_3		α-Cr_2O_3	
	Band gap (eV)	M (μB)	Band gap (eV)	M (μB)
5.0 eV	1.86	4.10	2.93	2.95
5.5 eV	2.05	4.15	3.09	2.98
6.0 eV	2.22	4.20	3.25	3.01
6.5 eV	2.41	4.25	3.38	3.03
7.0 eV	2.59	4.30	3.48	3.06
Experimental data	2.1-2.2[a,b]	4.9[a]	3.4[c]/3.1[d]	2.76[c]

[a] Reference [1]
[b] Reference [2]
[c] Reference [3]
[d] Reference [4]

2.Different spin configurations of Cr-doped α-Fe_2O_3 thin films

In the present study, two Fe atoms which have opposite magnetic moments were substituted by Cr atoms. We checked different magnetic orderings for the Cr-doped α-Fe_2O_3 thin films. Take model 2 as an example, Figure S1 shows four spin configurations, (a) and (b) are anti-ferromagnetic (AFM) states, (c) and (d) are ferromagnetic (FM) states. The results suggest that the spin configuration (a), in which two Cr atoms showing the same spin configurations with Fe atoms in the same octahedral layer is the most energetically stable. As a result, we only considered the magnetic ordering (a) in the present study.

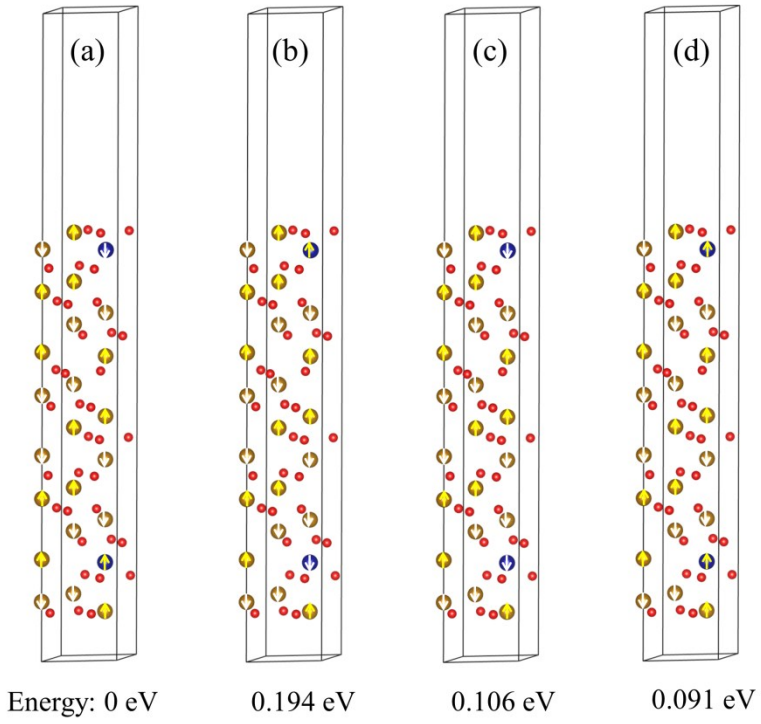

Figure S1. Different spin configurations of Cr-doped α-Fe_2O_3 (model 2) thin films. The up (down) arrows denote spin-up (-down) configurations for Fe or Cr atoms. (a) and (b) are AFM states, (c) and (d) are FM states.

3.The work function of the films

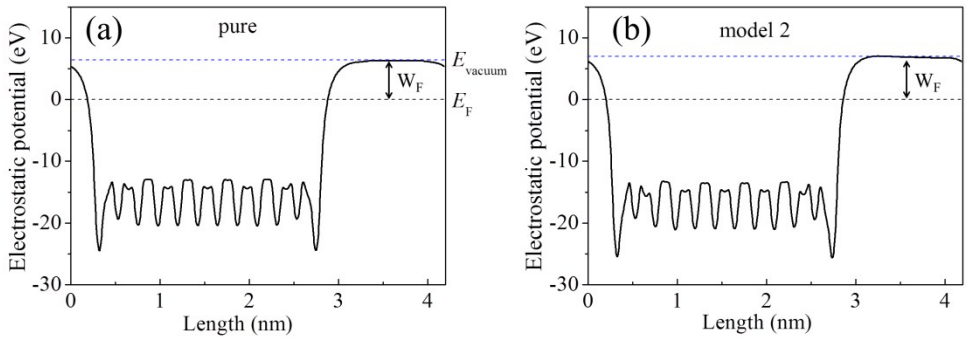

Figure S2. The calculated electrostatic potential of (a) the pure 1×1×2 α-Fe_2O_3 thin film and Cr-doped model 2. Work function (W_F) is the energy difference between the vacuum level E_{vacuum} and the Fermi level E_F of the system.

References:

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