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A sensitive material for optical fiber sensor —— $Dy_8Fe_{16-x}Co_x$ (x=0,2,3): First-principle calculations

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Introduction

Magnetic field is everywhere. In recent years, detecting magnetic field has become an important research direction. Magnetic field detection is widely used in medical treatment, power detection, aerospace and other fields. $DyFe_2$ as a photosensitive material can be combined with optical fiber to form an optical fiber sensor. In order to improve the sensitivity of optical sensors, a single transition metal Co doped $DyFe_2$ intermetallic compound is proposed in this paper. The physical properties of two concentrations of Co doped $DyFe_2$ compounds and intrinsic $DyFe_2$ compounds are comprehensively studied by first principles.

Results & Discussion

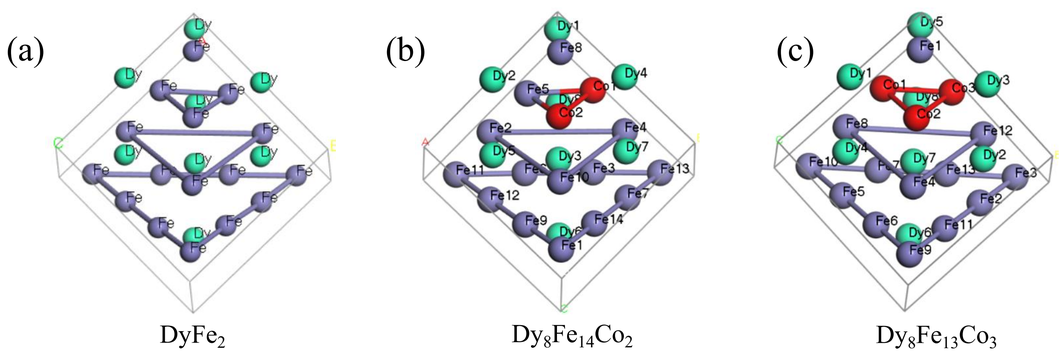

Fig. 1. The crystal structure of $DyFe_2$, $Dy_8Fe_{14}Co_2$ and $Dy_8Fe_{13}Co_3$

Electronic Properties

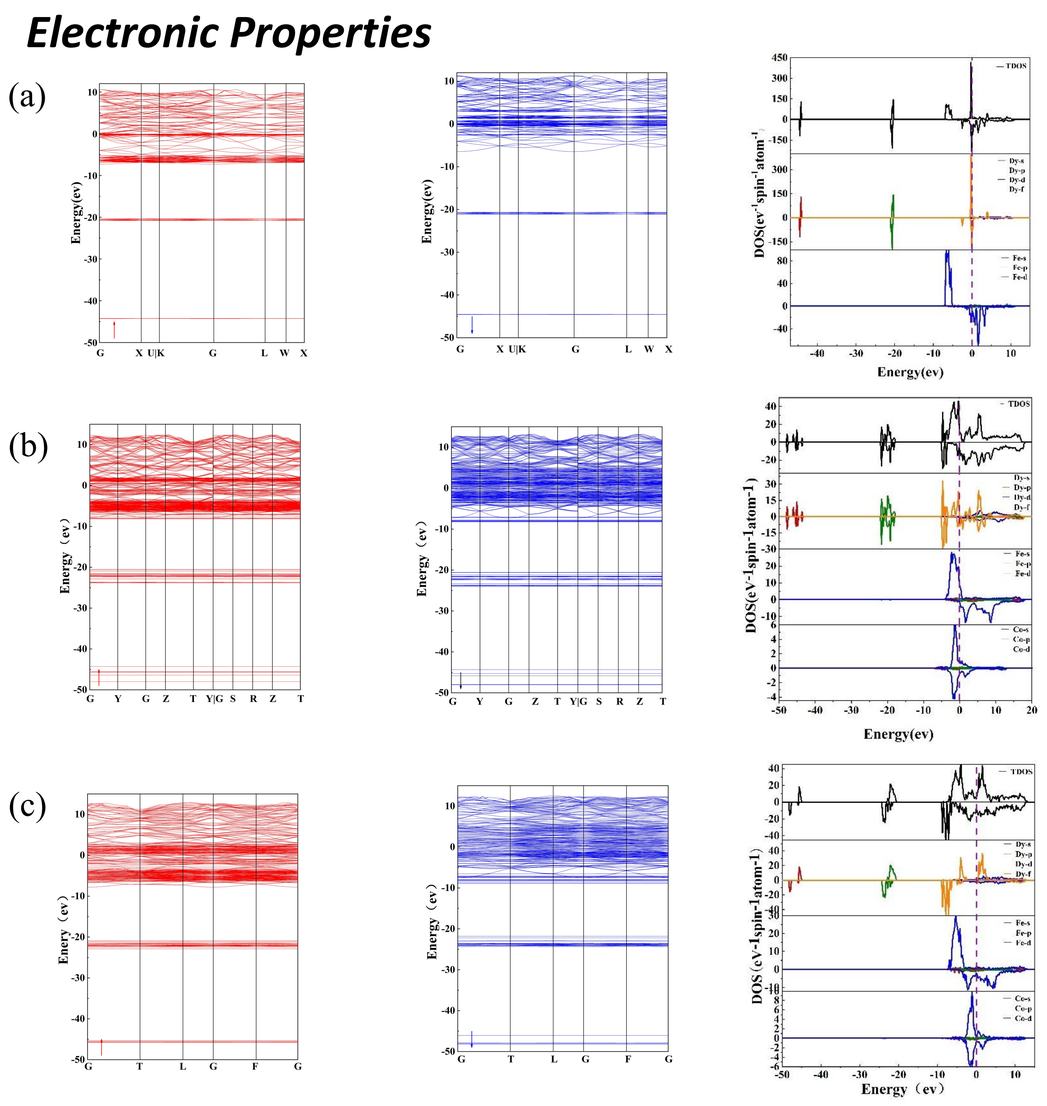

Fig. 2. The electrical properties of the $DyFe_2$, $Dy_8Fe_{14}Co_2$ and $Dy_8Fe_{13}Co_3$

The energy band and the density of states show the same metal characteristics, and it is found that the doping of Co will improve the activity of electrons, thus generating new impurity bands.

Magnetic Properties

Table I . The magnetic moment of total and partial about $DyFe_2$

	s	p	d	f	total
Dy_{1-8}	-0.034	-	-0.036	2.104	2.034
Fe_{1-16}	0.009	-0.024	3.100	-	3.086
tot	-0.124	-0.381	49.315	16.831	65.641

Table III . The magnetic moment of total and partial about $Dy_8Fe_{13}Co_3$

	s	p	d	f	total
$Dy_{1/3/5}$	-0.051	-0.024	-0.402	-4.983	-5.459
$Dy_{2/4/8}$	-0.048	-0.030	-0.384	-4.980	-5.442
Dy_6	-0.035	-0.020	-0.276	-1.451	-1.783
Dy_7	-0.071	-0.023	-0.447	-4.988	-5.539
Fe_1	0.013	-0.032	3.113	-	3.093
$Fe_{2/5/6/7/11/13}$	0.013	-0.052	3.052	-	3.013
$Fe_{3/9/10}$	0.004	-0.049	3.061	-	3.016
$Fe_{4/8/12}$	0.009	-0.027	3.032	-	3.014
$Co_{1/2/3}$	-0.019	-0.096	0.455	-	0.340
tot	-0.331	-1.063	37.984	-36.338	0.252

Table II . The magnetic moment of total and partial about $Dy_8Fe_{14}Co_2$

	s	p	d	f	total
$Dy_{1/2}$	-0.020	-0.007	-0.118	2.640	2.495
$Dy_{3/4}$	-0.049	-0.017	-0.371	-4.978	-5.415
$Dy_{5/8}$	-0.009	-0.016	-0.087	4.936	4.824
Dy_6	-0.029	-0.003	-0.147	0.055	-0.125
Dy_7	-0.049	-0.021	-0.424	-4.979	-5.473
$Fe_{1/7/13/14}$	0.011	-0.031	3.116	-	3.095
$Fe_{2/11}$	0.005	-0.007	2.983	-	2.982
$Fe_{3/4/9/10}$	0.012	-0.012	3.020	-	3.012
$Fe_{5/8}$	0.013	-0.007	3.029	-	3.035
$Fe_{6/12}$	0.013	-0.007	3.035	-	3.042
$Co_{1/2}$	-0.020	-0.079	0.382	-	0.283
tot	-0.119	-0.511	41.680	0.272	41.321

In the study of magnetism, this paper found an interesting phenomenon. Doping Co on the basis of breaking the triangle symmetry will make the same electron orbit of the same element produce different magnetic moments.

Optical Properties

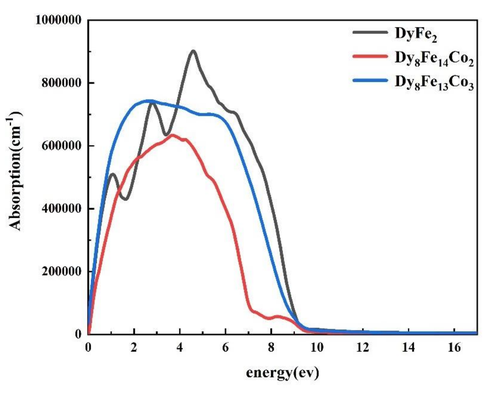

Fig. 3. Absorption spectra of $Dy_8Fe_{16-x}Co_x$ (x=0,2,3)

From the change between absorption intensity and energy, it can be found that the compound doped with Co can inhibit the two absorption peaks of intrinsic $DyFe_2$. And a red shift phenomenon occurs in the light absorption spectrum in the ultraviolet region.

Conclusion

Acknowledgement / National Natural Science Foundation of China (52102164)

In this paper, the structural, electrical and magnetic properties of $Dy_8Fe_{16-x}Co_x$ compound have been studied by GGA + U method. The above research has laid a foundation for understanding the basic physical properties of $Dy_8Fe_{16-x}Co_x$. Researchers can take corresponding measures to modify the optical fiber sensor of $Dy_8Fe_{16-x}Co_x$ compound. So as to improve the performance of the sensor and expand the application field of the sensor.