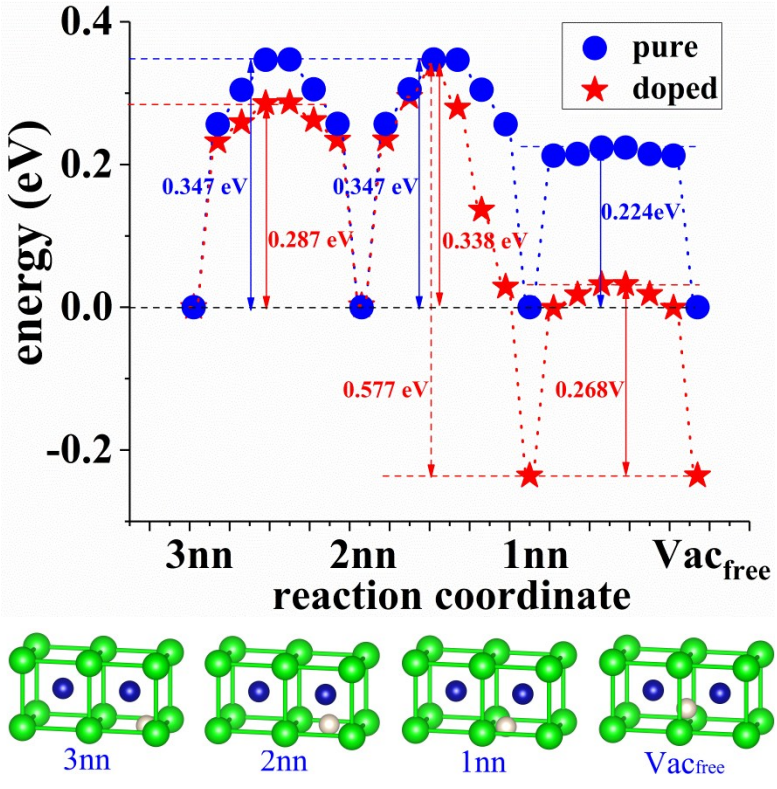
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effect of doping Ti on the vacancy trapping mechanism for the helium in ZrCo from first principles

Qingqing Wang,[a] Xianggang Kong,[b] You Yu,[b] Huilei Han,[c] Ge Sang,[#d] Guanghui Zhang,[d] Yougen Yi[e] and Tao Gao[*a]

Table of contents



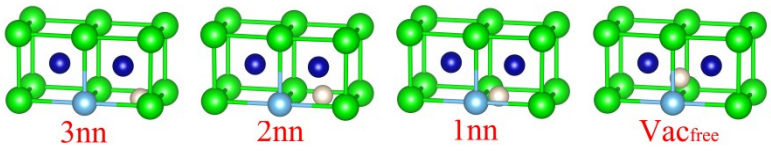


Fig. S1 Energetic barrier profiles and migration pathways: a single He atom migration from a remote interstitial site to a vacancy-free (Vac_{free}) in pure and doped ZrCo

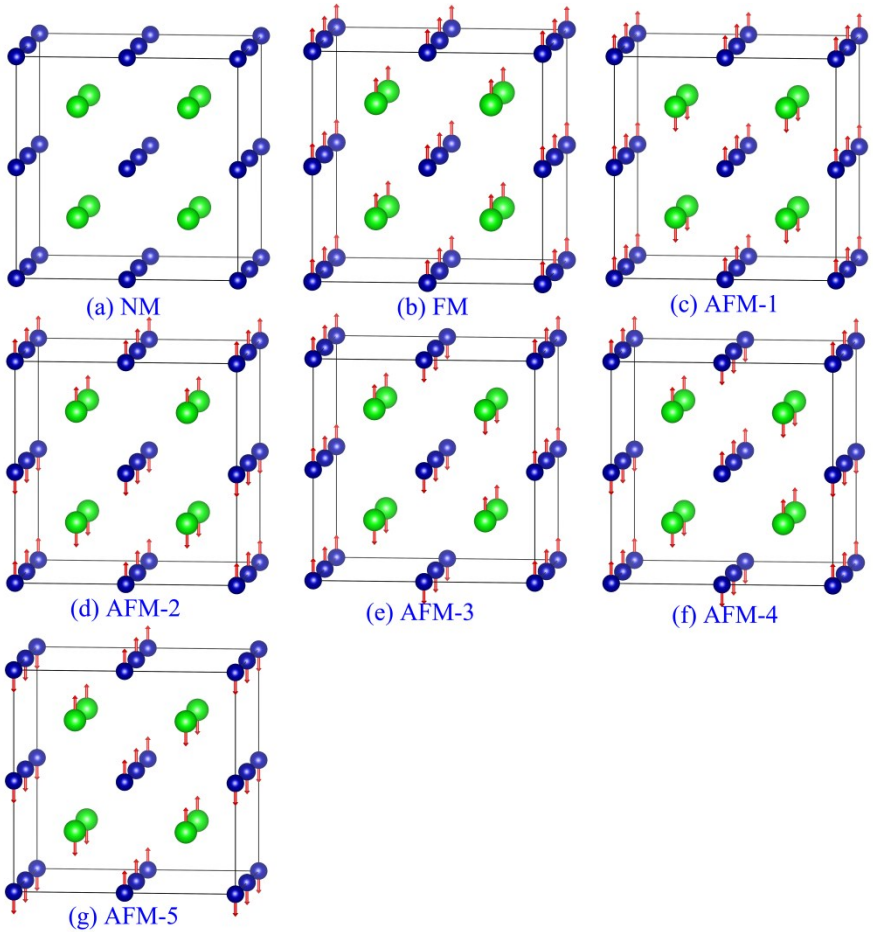


Fig. S2 The structural diagram of ZrCo in different magnetism

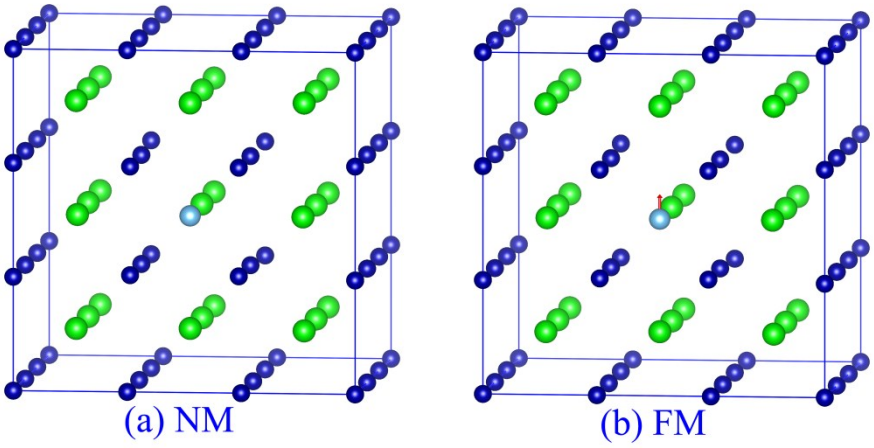


Fig. S3 The structural diagram of Ti-doped ZrCo in different magnetism

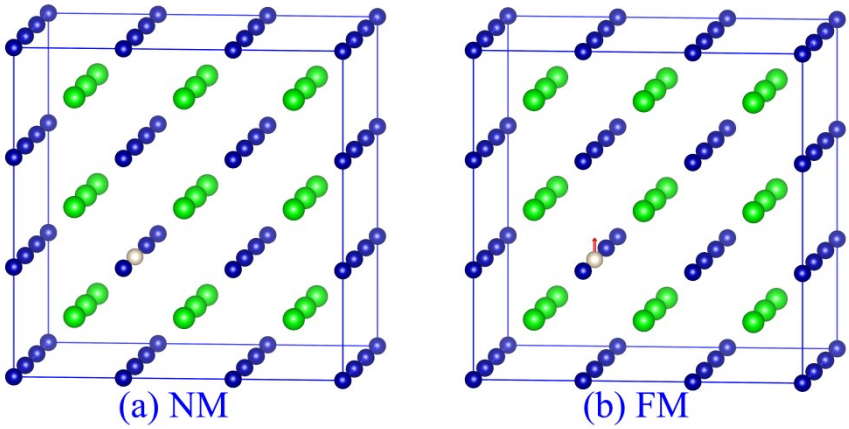


Fig. S4 The structural diagram of He_{sub} in different magnetism in ZrCo

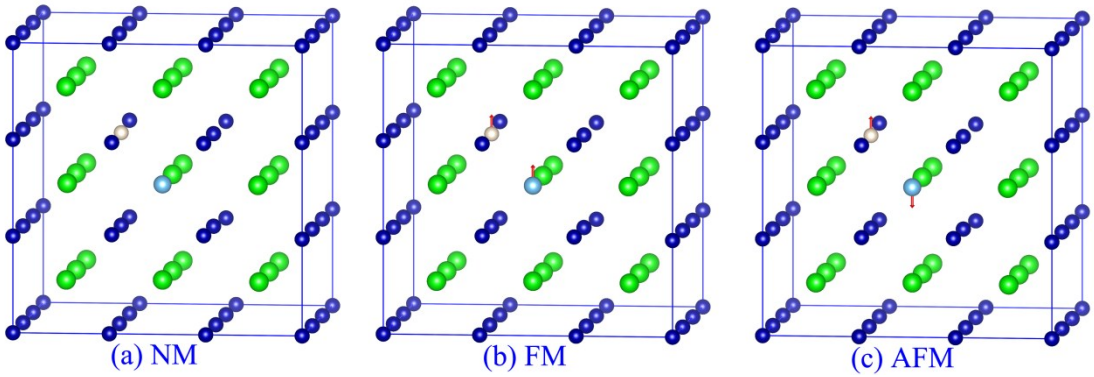


Fig. S5 The structural diagram of He_{sub} in different magnetism in Ti-doped ZrCo

Table S1. The relative energies of ZrCo of different magnetism

Magnetism*	ΔE(eV)
NM	0.000
FM	0.051
AFM-1	0.015
AFM-2	5E-08
AFM-3	7E-07
AFM-4	0.001
AFM-5	5E-07

The 'NM', 'FM', and 'AFM' refer to 'non-magnetic', 'ferromagnetic' and 'antiferromagnetic', respectively. '1-5' refer to five different antiferromagnetic states, as shown in Fig. S2.

Table S2. The relative energies of Ti-doped ZrCo of different magnetism

Magnetism*	ΔE(eV)
NM	0.000
FM	0.001

Table S3. The relative energies of He_{sub} of different magnetism in the ZrCo system

Magnetism*	ΔE(eV)
NM	0.000
FM	0.001

Table S4. The relative energies of He_{sub} of different magnetism in the Ti-doped ZrCo system

Magnetism*	ΔE(eV)
NM	0.000
FM	0.045
AFM	0.044