Electronic Supplementary Information

Insight of structural stability and helium diffusion behavior of Fe-Cr alloys from first-principles

Lei Wan,[a] Qingqing Wang,[a] Xiaoqiu Ye,[b] Xingzhong Cao,[c] Shuoxue Jin[c] and Tao Gao*[ad]

[a]Institute of Atomic and Molecular Physics, Sichuan University, Chengdu, Sichuan 610065, P. R. China. E-mail: gaotao@scu.edu.cn.

[b]Science and Technology on Surface Physics and Chemistry Laboratory, Mianyang, Sichuan 621907, P. R. China.

[c]Institute of High Energy Physics, Chinese Academy of Science, Beijing 100049, P. R. China.

[d]Key Laboratory of High Energy Density Physics and Technology of Ministry of Education, Sichuan University, Chengdu, Sichuan 610064, P. R. China. E-mail: gaotao@scu.edu.cn.

†Electronic supplementary information (ESI) available.

*Corresponding author. E-mail: gaotao@scu.edu.cn

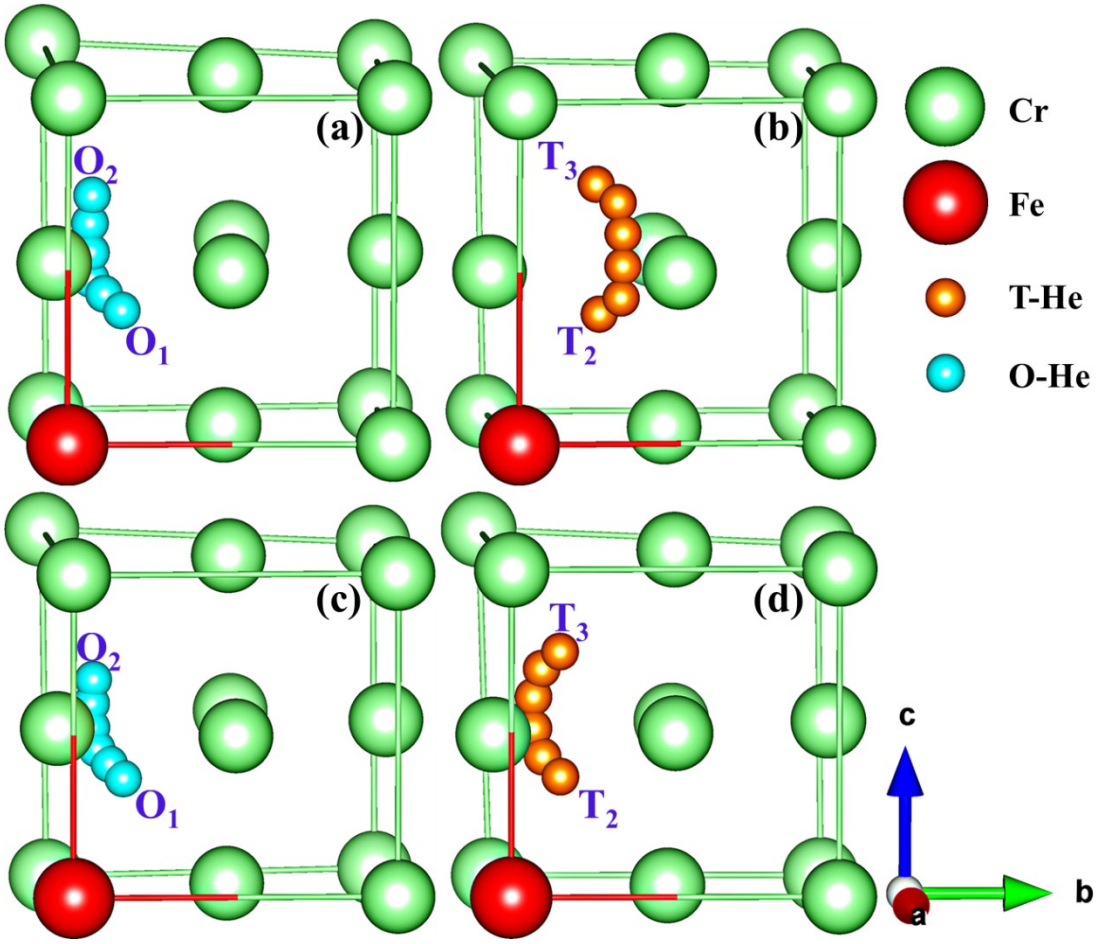

Figure S1. The structure diagrams of He migration between tetrahedral interstitials (Figures S1b and 1d) and octahedral interstitials (Figures S1a and 1c) of S_1 in AFM and NM states. (a) and (c) denote the structures of $O_1 \rightarrow O_2$ in the AFM and NM states. (b) and (d) indicate the structures of $T_2 \rightarrow T_3$ in the AFM and NM states, respectively. "T-He" and "O-He" represent the He atoms in tetrahedral and octahedral interstitials, respectively.

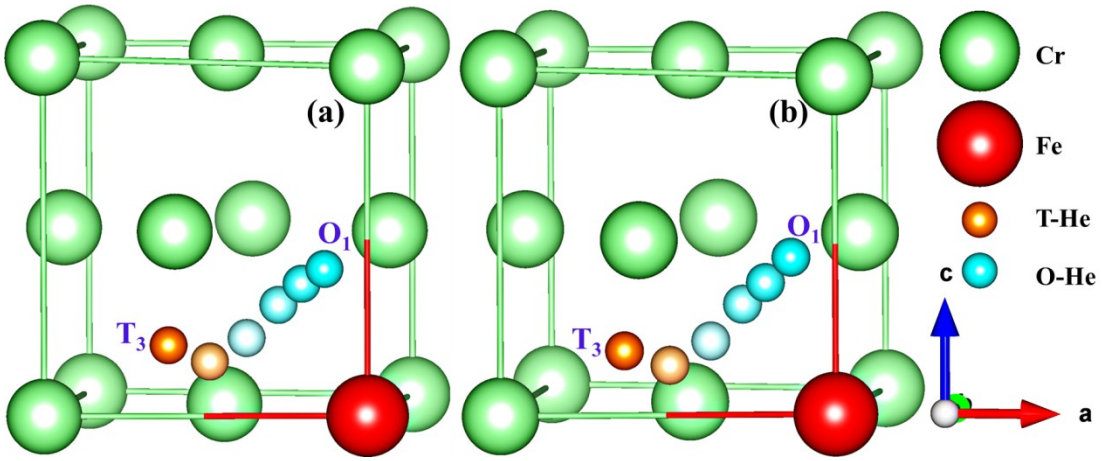

Figure S2. The structure diagrams of He migration between tetrahedral (T_3) and octahedral (O_1) interstitials of S_1 in AFM (Figure S2a) and NM (Figure S2b) states. "T-He" and "O-He" represent

the He atoms in tetrahedral and octahedral interstitials, respectively.

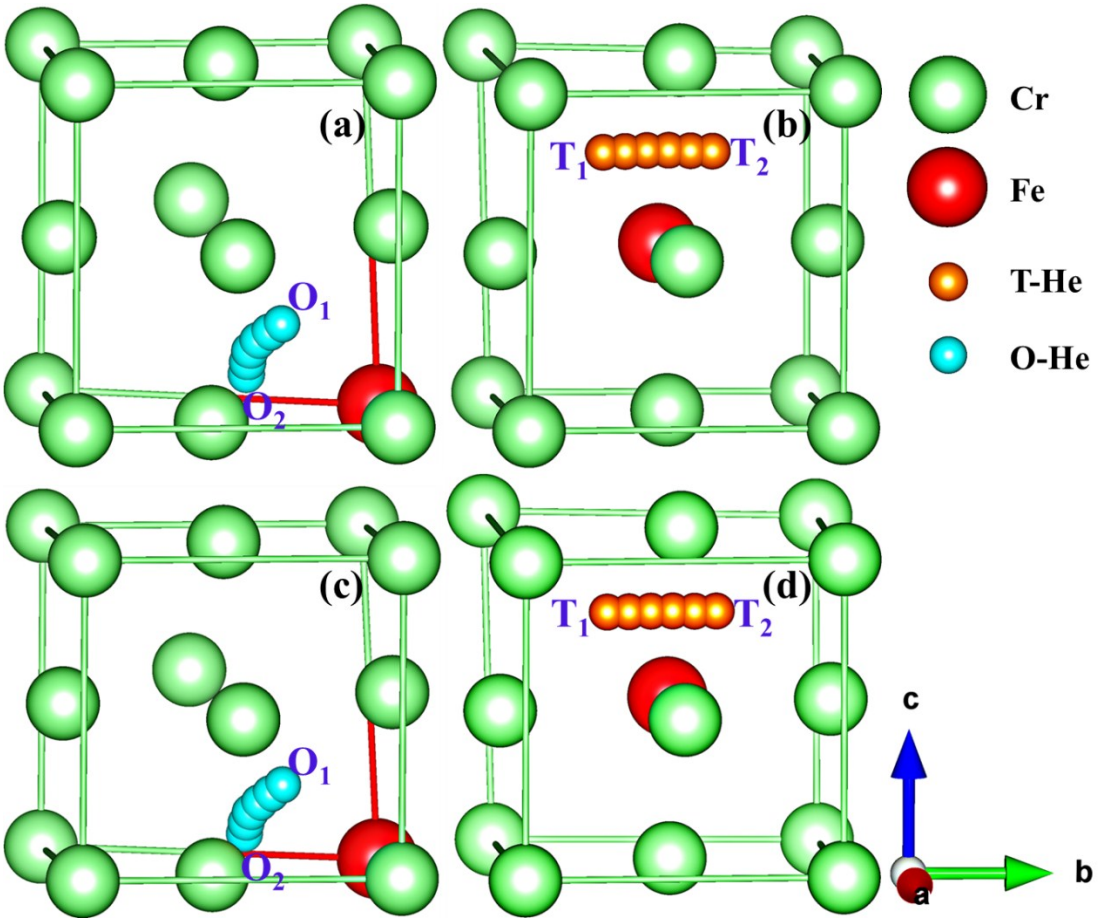

Figure S3. The structure diagrams of He migration between tetrahedral interstitials (Figures S3b and 3d) and octahedral interstitials (Figures S3a and 3c) of S_2 in AFM and NM states. (a) and (c) denote the structures of $O_1 \rightarrow O_2$ in the AFM and NM states. (b) and (d) indicate the structures of $T_2 \rightarrow T_3$ in the AFM and NM states, respectively. "T-He" and "O-He" represent the He atoms in tetrahedral and octahedral interstitials, respectively.

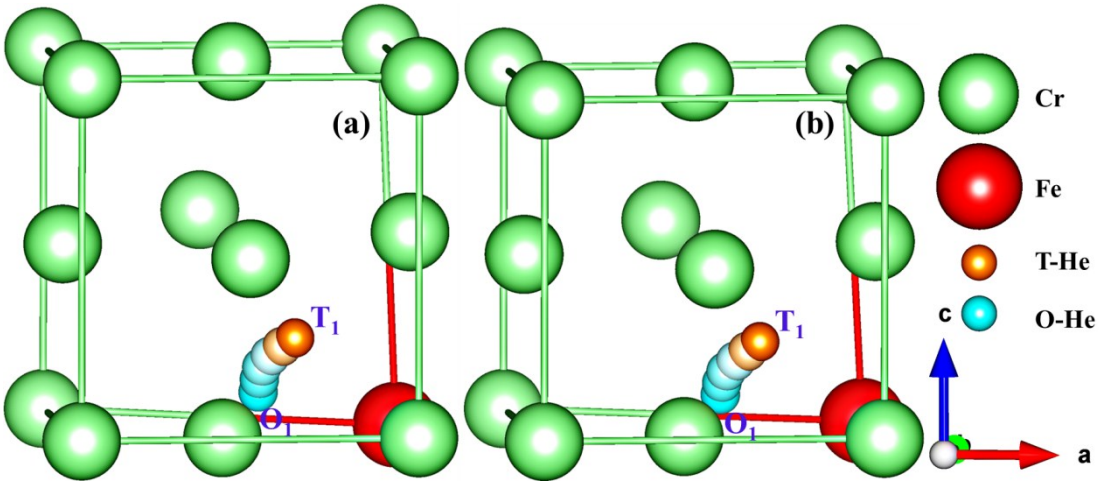

Figure S4. The structure diagrams of He migration between tetrahedral (T_1) and octahedral (O_1) interstitials of S_2 in AFM (Figure S4a) and NM (Figure S4b) states. "T-He" and "O-He" represent the He atoms in tetrahedral and octahedral interstitials, respectively.

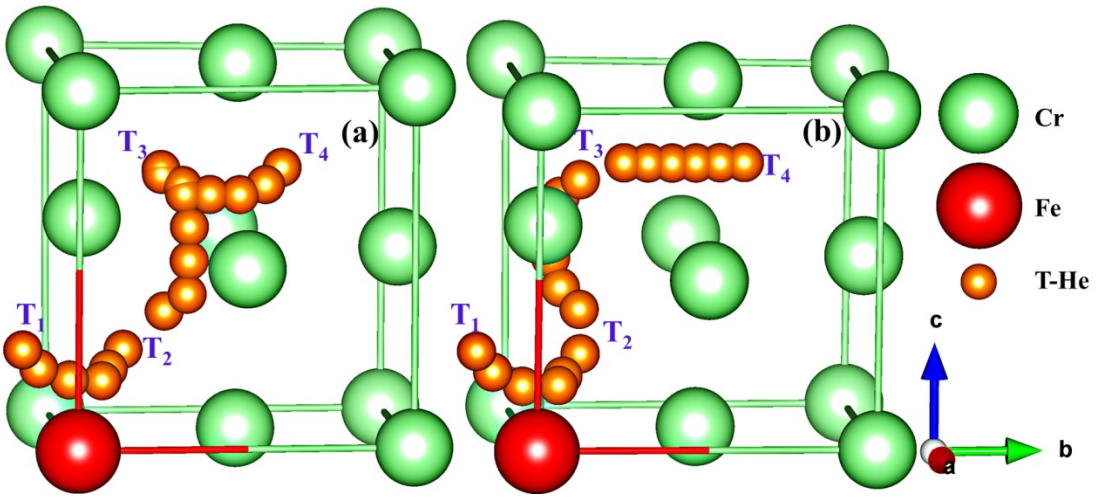

Figure S5. The structure diagrams of He migration between tetrahedral interstitials ($T_1 \rightarrow T_2 \rightarrow T_3 \rightarrow T_4$) of S_1 in AFM (Figure S5a) and NM (Figure S5b) states. "T-He" represents the He atoms in tetrahedral interstitials.

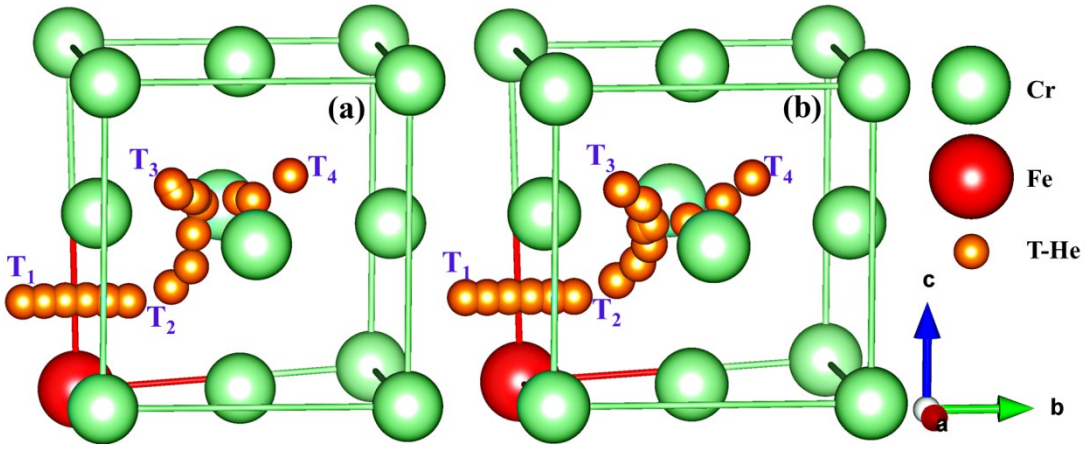

Figure S6. The structure diagrams of He migration between tetrahedral interstitials ($T_1 \rightarrow T_2 \rightarrow T_3 \rightarrow T_4$) of S_2 in AFM (Figure S6a) and NM (Figure S6b) states. "T-He" indicates the He atoms in tetrahedral interstitials.

Table S1 The Bader charges of S_1 and its bulk γ-Fe in AFM and NM states. "Doped" means Fe–Cr alloys structure. "Δ" indicates the difference of Bader charge after substitution.

site	Mag.	Atom	Pure (|e|)	Doped (|e|)	Δ (|e|)
		Fe_1	8.000	8.033	0.033
		Fe_2		8.052	0.052

		Fe_3		8.032	0.032
		Fe_8		8.031	0.031
		Fe_{10}		8.049	0.049
		Fe_{16}		8.033	0.033
		Fe_{19}		8.032	0.032
		Fe_{24}		8.031	0.031
		Cr	–	5.555	–0.445
		total	256.000	254.000	
	NM	Fe_1	8.000	8.036	0.036
		Fe_2		8.037	0.037
		Fe_3		8.037	0.037
		Fe_8		8.037	0.037
		Fe_{10}		8.036	0.036
		Fe_{16}		8.037	0.037
		Fe_{19}		8.036	0.036
		Fe_{24}		8.038	0.038
		Cr	–	5.532	–0.468
		total	256.000	254.000	

Table S2 The Bader charges of S_2 and its pure γ-Fe alloy in AFM and NM states. "Doped" denotes Fe–Cr alloy structure. "Δ" represents the difference of Bader charge after substitution.

site	Mag.	Atom	Pure (|e|)	Doped (|e|)	Δ (|e|)
S_2	AFM	Fe_6	8.000	8.031	0.031
		Fe_{11}		8.031	0.031
		Fe_{14}		8.031	0.031
		Fe_{15}		8.031	0.031
		Fe_{20}		8.050	0.050
		Fe_{22}		8.031	0.031
		Fe_{24}		8.050	0.050
		Fe_{27}		8.031	0.031
		Fe_{28}		8.050	0.050
		Fe_{29}		8.031	0.031
		Fe_{30}		8.031	0.031
		Fe_{31}		8.050	0.050
		Cr	–	5.554	–0.446
		total	256.000	254.000	
		Fe_6	8.000	8.036	0.036

		Fe_{11}		8.036	0.036
		Fe_{14}		8.036	0.036
		Fe_{15}		8.036	0.036
		Fe_{20}		8.036	0.036
		Fe_{22}		8.036	0.036
		Fe_{24}		8.036	0.036
		Fe_{27}		8.036	0.036
		Fe_{28}		8.036	0.036
		Fe_{29}		8.036	0.036
		Fe_{30}		8.036	0.036
		Fe_{31}		8.036	0.036
		Cr	–	5.532	–0.468
		total	256.000	254.000	