Supporting information

Crystal Structure Prediction Approach to Explore the Iron Carbide Phases: Novel Crystal Structures and Unexpected Magnetic Properties

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Table S1. A summary of DFT optimized structural parameters of iron carbides obtained or proposed by experimentalists and theorists (The calculation of formation energy is based on α-Fe and graphite).

Compound	Space group	Lattice constants(Å)		Atom position (Wyckoff position)	Formation energy (eV/atom)
α'-$Fe_{16}C_2$[1]	I4/mmm	a=5.668	α=90	Fe(4e) 0.0,0.0,0.706	0.042
		b=5.668	β=90	Fe(8h) 0.757,0.243,0.0	
		c=6.242	γ=90	Fe(4d) 0.0,0.5,0.75	
				C(2a) 0.0,0.0,0.0	
γ'-Fe_4C [2]	P-43m	a=3.719	α=90	Fe(4e) 0.277,0.277,0.277	0.585
		b=3.719	β=90	C(1a) 0,0,0	
		c=3.719	γ=90		
γ''-Fe_4C	Pm-3m	a=3.762	α=90	Fe(1a) 0,0,0	0.111
		b=3.762	β=90	Fe(3c) 0.5,0.5,0	
		c=3.762	γ=90	C(1b) 0.5,0.5,0.5	
θ-Fe_3C [3]	Pnma	a=5.022	α=90	Fe(8d) 0.822,0.568,0.667	0.043
		b=6.718	β=90	Fe(4c) 0.036,0.25,0.838	
		c=4.469	γ=90	C(4c) 0.877,0.25,0.437	
ε-Fe_3C [4]	$P6_322$	a=4.641	α=90	Fe(6g) -0.322,-0.322,0	0.045
		b=4.641	β=90	C(2d) 0.333,-0.333,0.75	
		c=4.303	γ=120		
Fe_3C[5]	P-31m	a=4.652	α=90	Fe(6k) 0.33,0,0.26	0.122
		b=4.652	β=90	C(2c) 0.667,0.333,1.0	
		c=4.274	γ=120		
χ-Fe_5C_2 [6]	C2/c	a=11.553	α=90	Fe(8f) 0.098,0.084,0.918	0.046
		b=4.499	β=97.591	Fe(8f) 0.215,0.583,0.811	
		c=4.982	γ=90	Fe(4e) 0,0.57,0.75	
				C(8f) 0.113,0.314,0.579	
h-Fe_7C_3 [7]	$P6_3mc$	a=6.813	α=90	Fe(2b) 0.333,0.667,0.811	0.068
		b=6.813	β=90	Fe(6c) 0.454,0.546,0.316	
		c=4.479	γ=120	Fe(6c) 0.122,0.878,-0.01	
				C(6c) 0.187,0.813,0.595	
o-Fe_7C_3	Pnma	a=4.507	α=90	Fe(8d) -0.248,0.067,0.015	0.051
		b=6.844	β=90	Fe(8d) -0.439,0.063,0.808	
		c=11.716	γ=90	Fe(4c) -0.205,0.25,0.199	
				Fe(4c) -0.226,0.25,0.412	
				Fe(4c) -0.42,0.25,0.628	
				C(8d) -0.459,0.026,0.353	
				C(4c) -0.031,0.25,0.562	
η-Fe_2C [8]	Pnnm	a=4.698	α=90	Fe(4g) 0.656,0.25,0.5	0.047
		b=4.273	β=90	C(2b) 0,0,0.5	

		c=2.82	γ=90		
ε-Fe_2C [9]	Pbcn	a=4.289	α=90	Fe(8d) -0.251,0.616,1.079	0.054
		b=5.466	β=90	C(4c) -0.5,0.364,1.25	
		c=4.841	γ=90		
Fe_2C [10]	P6/mmm	a=3.597	α=90	Fe(2c) 0.333,0.667,0	1.189
		b=3.597	β=90	C(1a) 0,0,0	
		c=2.625	γ=120		
γ'-FeC[11,12]	Fm-3m	a=3.994	α=90	Fe(4b) 0.5,0,0	0.615
		b=3.994	β=90	C(4a) 0,0,0	
		c=3.994	γ=90		

Table S2. A summary of DFT optimized structural parameters of iron carbides obtained by our structure prediction (The calculation of formation energy is based on α-Fe and graphite).

Compound	Space group	Lattice constants(Å)		Atom position (wyckoff position)	Formation energy (eV/atom)
Fe_7C	P-1	a=4.7073	α=76.441	Fe(2i) -0.172,0.244,-0.147	0.051
		b=4.7345	β=81.937	Fe(2i) 0.353,0.708,-0.119	
		c=8.8929	γ=65.234	Fe(2i) 0.246,0.246,-0.002	
				Fe(2i) 0.608,0.755,0.288	
				Fe(2i) 0.098,0.253,0.279	
				Fe(2i) -0.066,0.286,0.551	
				Fe(2i) 0.464,0.751,0.577	
				C(2i) -0.145,1.001,0.285	
Fe_6C	P1	a=4.693	α=83.018	Fe(1a) 0.347,0.629,0.693	0.055
		b=5.104	β=79.094	Fe(1a) 0.718,0.755,0.359	
		c=6.535	γ=83.118	Fe(1a) 0.719,0.256,0.359	
				Fe(1a) 0.348,0.126,0.694	
				Fe(1a) 0.23,0.466,0.382	
				Fe(1a) 0.243,0.973,0.336	
				Fe(1a) 0.509,0.215,0.025	
				Fe(1a) 0.822,0.409,0.719	
				Fe(1a) 0,0,0	
				Fe(1a) 0.012,0.474,0.024	
				Fe(1a) 0.84,0.887,0.695	
				Fe(1a) 0.513,0.712,0.021	
				C(1a) 0.029,0.181,0.533	
				C(1a) 0.115,0.727,0.186	
Fe_5C	C2/m	a=2.625	α=90	Fe(4i) 0.319,0.203,0	0.079
		b=12.288	β=90	Fe(4i) -0.004,0.61,0	
		c=3.979	γ=90.963	Fe(2c) -0.5,0.5,-0.5	

				C(2d) -0.5,0.5,0	
Fe_4C	Fdd2	a=8.978	α=90	Fe(16b) -0.58,0.124,0.156	0.069
		b=8.76	β=90	Fe(16b) -0.338,0.117,0.919	
		c=5.291	γ=90	C(8a) -0.25,0.25,0.668	
Fe_7C_2	C2	a=11.748	α=90	Fe(4c) -0.147,0.206,-0.148	0.060
		b=6.802	β=90	Fe(4c) 0.142,0.286,0.192	
		c=4.591	γ=86.575	Fe(4c) 0.21,0.422,0.67	
				Fe(4c) 0.069,0.638,0.352	
				Fe(4c) 0.286,1.062,0.836	
				Fe(4c) 0.074,0.864,0.67	
				Fe(2b) 0,0.5,0.829	
				Fe(2a) 0,1,0.194	
				C(4c) 0.285,0.318,1.011	
				C(4c) -0.001,0.248,0.009	
Fe_3C	find θ-Fe_3C [3]				
Fe_5C_2	find χ-Fe_5C_2 [6]				
Fe_7C_3	find h-Fe_7C_3 [7]				
$Fe_{11}C_5$	P1	a=8.441	α=95.875	Fe(1a) 0.259,0.28,0.658	0.085
		b=7.219	β=89.152	Fe(1a) 0.436,0.569,0.851	
		c=5.096	γ=83.569	Fe(1a) 0.251,0.178,0.159	
				Fe(1a) 0.325,0.813,0.236	
				Fe(1a) 0.53,0.198,0.943	
				Fe(1a) 0.421,0.45,0.331	
				Fe(1a) 0.341,0.93,0.744	
				Fe(1a) 0.077,0.018,0.505	
				Fe(1a) 0.166,0.635,0.583	
				Fe(1a) 0.155,0.555,0.07	
				Fe(1a) 0.987,0.276,0.904	
				Fe(1a) 0.071,0.893,0.989	
				Fe(1a) 0.995,0.371,0.41	
				Fe(1a) 0.516,0.085,0.422	
				Fe(1a) 0.806,0.107,0.238	
				Fe(1a) 0.693,0.358,0.62	
				Fe(1a) 0.79,0.992,0.713	
				Fe(1a) 0.901,0.744,0.324	
				Fe(1a) 0.882,0.626,0.802	
				Fe(1a) 0.603,0.718,0.52	
				Fe(1a) 0.624,0.836,0.035	
				Fe(1a) 0.715,0.478,0.136	
				C(1a) 0.38,0.689,0.539	
				C(1a) 0.037,0.13,0.182	
				C(1a) 0.336,0.375,0.994	
				C(1a) 0.706,0.906,0.371	

				C(1a) 0.659,0.597,0.827	
				C(1a) 0.885,0.2,0.6	
				C(1a) 0.615,0.287,0.281	
				C(1a) 0.938,0.511,0.114	
				C(1a) 0.986,0.816,0.658	
				C(1a) 0.429,0.996,0.079	
Fe_2C	find η-Fe_2C [8]				
Fe_7C_4	C2/m	a=7.033	α=90	Fe(4i) -0.276,0.15,0.5	0.131
		b=9.828	β=90	Fe(4i) -0.919,0.256,0.5	
		c=2.758	γ=90.677	Fe(4i) -0.659,0.452,0.5	
				Fe(2d) -0.5,0,0	
				C(4i) -0.835,0.405,1	
				C(4i) -1.078,0.15,1	
Fe_5C_3	C2/c	a=5.883	α=90	Fe(8f) -0.161,0.08,0.464	0.156
		b=9.964	β=90	Fe(8f) 0.052,-0.189,0.319	
		c=9.868	γ=83.287	Fe(8f) -0.144,0.078,0.186	
				Fe(8f) 0.279,0.429,0.342	
				Fe(8f) 0.048,-0.199,0.027	
				C(8f) -0.347,0.622,0.468	
				C(8f) -0.154,0.374,0.631	
				C(8f) -0.38,0.616,0.174	
Fe_3C_2	Cmcm	a=6.573	α=90	Fe(4c) -0.75,0.733,0	0.148
		b=6.904	β=90	Fe(8g) -0.25,0.776,0.163	
		c=7.535	γ=90	Fe(4a) -0.5,0.5,0.5	
				Fe(8e) -0.5,0.5,-0.165	
				C(8g) -0.25,0.553,0.314	
				C(8f) -1.04,0.709,0	
Fe_7C_5	C2	a=5.762	α=90	Fe(4c) 0.141,-0.714,-1.286	0.162
		b=8.062	β=90	Fe(4c) -0.417,-0.866,-1.266	
		c=4.498	γ=81.522	Fe(4c) -0.271,-0.578,-1.269	
				Fe(2a) 0,-1,-1.27	
				C(4c) -0.236,-0.421,-0.597	
				C(4c) -0.131,-0.791,-1.445	
Fe_4C_3	Cmcm	a=8.926	α=90	Fe(8e) -0.5,-0.251,0.5	0.159
		b=5.084	β=90	Fe(8g) -0.239,0.255,0.75	
		c=5.223	γ=90	C(8f) -0.16,0,0.494	
				C(4c) -0.564,0,0.75	
Fe_5C_4	C2/m	a=5.085	α=90	Fe(4i) 0.811,0.303,0.5	0.190
		b=11.105	β=90	Fe(4i) 0.609,0.098,0.5	
		c=2.672	γ=84.515	Fe(2a) 0.808.0.171,0	
				C(4i) 0.249,0.065,0.5	
				C(4i) 0.808,0.171,0	
Fe_6C_5	Imm2	a=13.548	α=90	Fe(4d) -0.288,0,-0.252	0.224

		b=2.63	β=90	Fe(4d) 0.041,0,-0.756	
		c=5.062	γ=90	Fe(4d) -0.124,0.5,-0.749	
				C(2b) -0.186,0,-0.5	
				C(2b) -0.392,0,-0.5	
				C(2a) -0.006,0.5,-0.5	
				C(2b) -0.253,0.5,0	
				C(2a) -0.067,0,-1	
Fe_7C_6	$P6_3/m$	a=7.038	α=90	Fe(12i) 0.417,0.125,-0.506	0.276
		b=7.038	β=90	Fe(2b) 0,0,0	
		c=5.037	γ=120	C(6h) 0.522,-0.378,-0.25	
				C(6h) 0.247,0.192,-0.25	
FeC	Pnnm	a=6.367	α=90	Fe(4g) -0.311,-0.102,0	0.297
		b=3.781	β=90	C(4g) -0.901,-0.897,-0.5	
		c=2.857	γ=90		

Table S3. (a) A summary of the elastic constants of the predicted iron carbides (unit: Gpa)

Compound	Fe_7C	Fe_6C	Fe_5C	Fe_4C	Fe_7C_2	θ-Fe_3C	χ-Fe_5C_2	o-Fe_7C_3	$Fe_{11}C_5$	η-Fe_2C
Space group	P-1	P1	C2/m	Fdd2	C2	Pnma	C2/c	Pnma	P1	Pnnm
Stability	yes	yes	yes	yes	yes	yes	yes	yes	yes	yes
C11	306	292	311	316	326	379	355	362	357	349
C22	304	347	337	282	311	395	350	428	322	404
C33	332	311	360	175	306	322	417	444	352	457
C44	80	73	80	79	61	11	152	121	105	118
C55	88	98	75	51	89	142	143	112	89	109
C66	107	90	81	78	89	137	44	67	99	148
C12	136	129	126	116	132	188	179	173	153	241
C13	134	129	108	151	148	154	142	171	151	189
C14	-11	0	0	0	0	0	0	0	-6	0
C15	21	1	0	0	0	0	-9	0	-9	0
C16	7	-23	-8	0	-4	0	0	0	-6	0
C23	135	123	123	44	156	219	157	173	163	213
C24	-10	1	0	0	0	0	0	0	-10	0
C25	-7	-2	0	0	0	0	24	0	-1	0
C26	-13	12	-34	0	-5	0	0	0	-2	0
C34	13	1	0	0	0	0	0	0	-4	0
C35	-12	-2	0	0	0	0	1	0	8	0
C36	-7	11	39	0	18	0	0	0	11	0
C45	3	25	15	0	-8	0	0	0	8	0
C46	-22	2	0	0	0	0	-9	0	-8	0
C56	5	0	0	0	0	0	0	0	-1	0

Table S3. (b) A summary of the elastic constants of the predicted iron carbides (unit: Gpa)

Compound	Fe_7C_4	Fe_5C_3	Fe_3C_2	Fe_7C_5	Fe_4C_3	Fe_5C_4	Fe_6C_5	Fe_7C_6	FeC
Space group	C2/m	C2/c	Cmcm	C2	Cmcm	C2/m	Imm2	$P6_3/m$	Pnnm
Stability	yes	yes	yes	yes	yes	yes	yes	yes	yes
C11	465	404	496	464	478	452	485	407	523
C22	445	272	517	631	803	626	512	407	666
C33	418	429	575	551	541	421	794	656	225
C44	170	119	157	171	188	222	213	198	159
C55	136	128	118	173	195	161	152	198	103
C66	89	98	203	196	150	213	164	126	126
C12	183	231	236	243	150	175	263	155	216
C13	163	172	119	149	199	221	178	148	187
C14	0	0	0	0	0	0	0	0	0
C15	0	0	0	0	0	0	0	0	0
C16	28	-60	0	10	0	18	0	0	0
C23	239	192	156	203	186	156	188	148	191
C24	0	0	0	0	0	0	0	0	0
C25	0	0	0	0	0	0	0	0	0
C26	15	9	0	109	0	102	0	0	0
C34	0	0	0	0	0	0	0	0	0
C35	0	0	0	0	0	0	0	0	0
C36	-18	-4	0	6	0	-21	0	0	0
C45	-4	19	0	10	0	-13	0	0	0
C46	0	0	0	0	0	0	0	0	0
`C56	0	0	0	0	0	0	0	0	0

Table S4. A summary of magnetic hyperfine fields of the predicted iron carbides (Mag means magnetic moment, unit B_{hf}: T, Mag: μ_B)

	Fe_7C	Fe_5C	Fe_4C	Fe_7C_2	θ-Fe_3C	χ-Fe_5C_2	o-Fe_7C_3	η-Fe_2C	Fe_7C_4
B_{hf}(Fe1)	-27.23	-30.84	-22.93	-25.26	-24.36	-24.38	-23.23	-18.04	-18.28
Mag(Fe1)	2.22	2.59	1.67	1.84	1.86	2.08	1.93	1.65	1.79
B_{hf}(Fe2)	-27.59	-23.53	-31.62	-22.31	-25.16	-21.44	-19.02		-17.61
Mag(Fe2)	2.01	1.64	2.39	1.78	1.96	1.65	1.71		1.88
B_{hf}(Fe3)	-32.66	-26.74		-25.15		-14.35	-23.13		-8.34
Mag(Fe3)	2.55	2.28		1.94		1.03	1.72		0.65
B_{hf}(Fe4)	-30.61			-23.76			-20.23		-15.35
Mag(Fe4)	2.39			1.87			1.68		1.37

B_{hf}(Fe5)	-29.69			-29.55			-17.66		
Mag(Fe5)	2.37			2.25			1.48		
B_{hf}(Fe6)	-27.83			-31.37					
Mag(Fe6)	1.96			2.32					
B_{hf}(Fe7)	-27.49			-25.25					
Mag(Fe7)	2.29			1.94					
B_{hf}(Fe8)				-23.5					
Mag(Fe8)				1.71					
Fe_6C				$Fe_{11}C_5$					
B_{hf}(Fe1)	-32.65	Fe9	-29.25	B_{hf}(Fe1)	-28.51	Fe9	-22.45	Fe17	-20.68
Mag(Fe1)	2.64	Fe9	2.02	Mag(Fe1)	2.49	Fe9	1.94	Fe17	1.92
B_{hf}(Fe2)	-30.04	Fe10	-27.93	B_{hf}(Fe2)	-16.43	Fe10	-22.63	Fe18	-15.85
Mag(Fe2)	2.45	Fe10	2.22	Mag(Fe2)	1.59	Fe10	1.94	Fe18	1.47
B_{hf}(Fe3)	-30.14	Fe11	-27.36	B_{hf}(Fe3)	-14.34	Fe11	-15.05	Fe19	-15.7
Mag(Fe3)	2.45	Fe11	2.23	Mag(Fe3)	1.3	Fe11	1.31	Fe19	1.53
B_{hf}(Fe4)	-29.41	Fe12	-28.49	B_{hf}(Fe4)	-22.22	Fe12	-22.34	Fe20	-17.44
Mag(Fe4)	2.26	Fe12	2.3	Mag(Fe4)	1.94	Fe12	1.88	Fe20	1.59
B_{hf}(Fe5)	-23.23			B_{hf}(Fe5)	-21.4	Fe13	-19.67	Fe21	-16.75
Mag(Fe5)	1.7			Mag(Fe5)	1.96	Fe13	1.7	Fe21	1.55
B_{hf}(Fe6)	-22.82			B_{hf}(Fe6)	-16.79	Fe14	-22.07	Fe22	-17.93
Mag(Fe6)	1.69			Mag(Fe6)	1.52	Fe14	1.84	Fe22	1.58
B_{hf}(Fe7)	-30.75			B_{hf}(Fe7)	-23.97	Fe15	-16.54		
Mag(Fe7)	2.57			Mag(Fe7)	1.98	Fe15	1.52		
B_{hf}(Fe8)	-27.43			B_{hf}(Fe8)	-19.21	Fe16	-16.87		
Mag(Fe8)	1.94			Mag(Fe8)	1.59	Fe16	1.53		
	Fe_5C_3	Fe_3C_2	Fe_7C_5	Fe_4C_3	Fe_5C_4	Fe_6C_5	Fe_7C_6	FeC	
B_{hf}(Fe1)	-9.72	-2.63	0	0	-3.33	-1.34	-2.77	-9.96	
Mag(Fe1)	0.9	0.36	0	0	0.48	0.06	0.21	1.1	
B_{hf}(Fe2)	-2.58	-0.04	0	0	-3.33	-2.29	-4.85		
Mag(Fe2)	-0.04	-0.08	0	0	0.48	0.19	0.43		
B_{hf}(Fe3)	-5.17	-0.61	0		0.55	-3.01			
Mag(Fe3)	0.32	0.01	0		-0.2	0.27			
B_{hf}(Fe4)	-13.8	-0.67	0		0.55				
Mag(Fe4)	1.71	0.05	0		-0.2				
B_{hf}(Fe5)	-4.92				2.71				
Mag(Fe5)	0.21				-0.4				

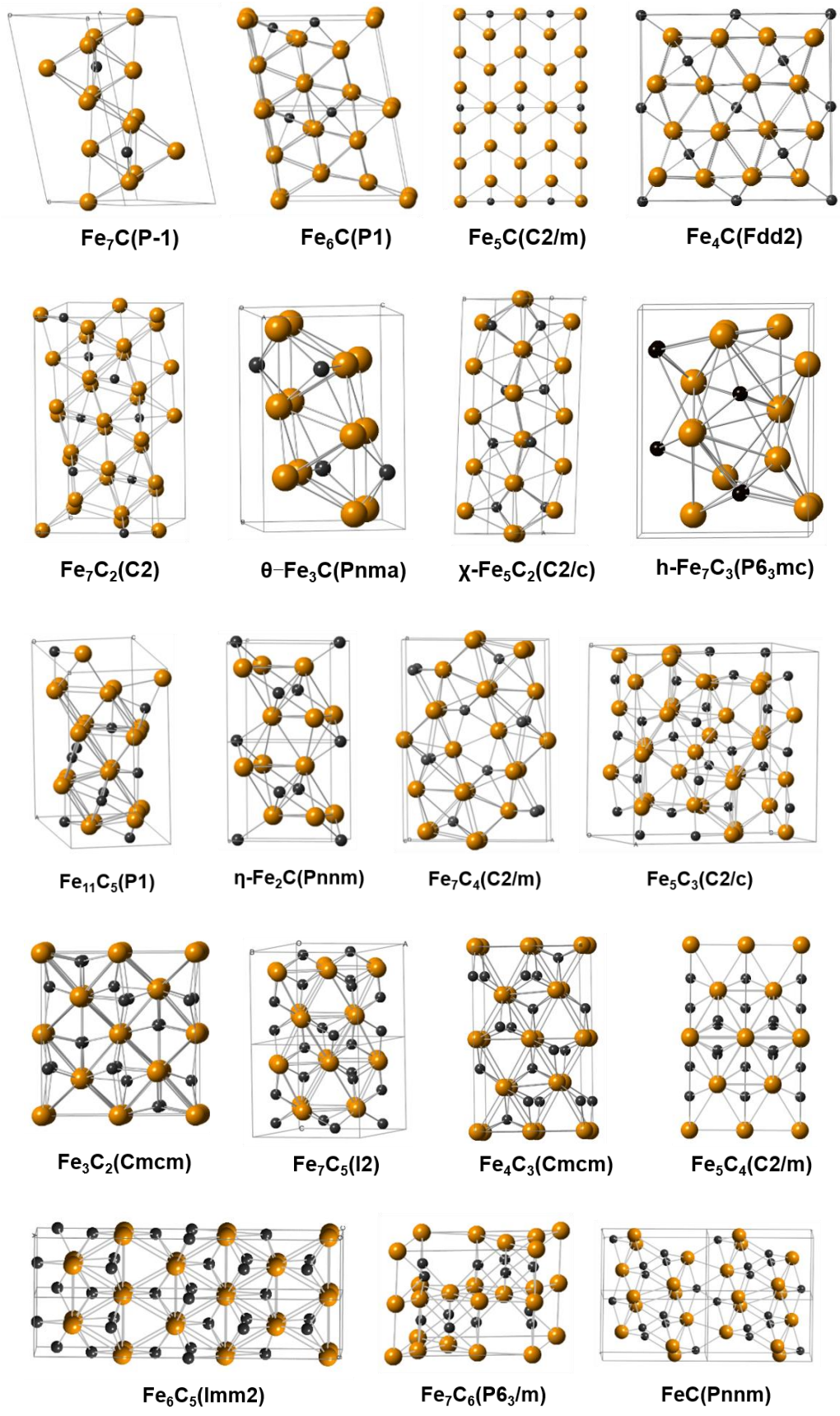


Figure S1. Crystal structures of the predicted iron carbides

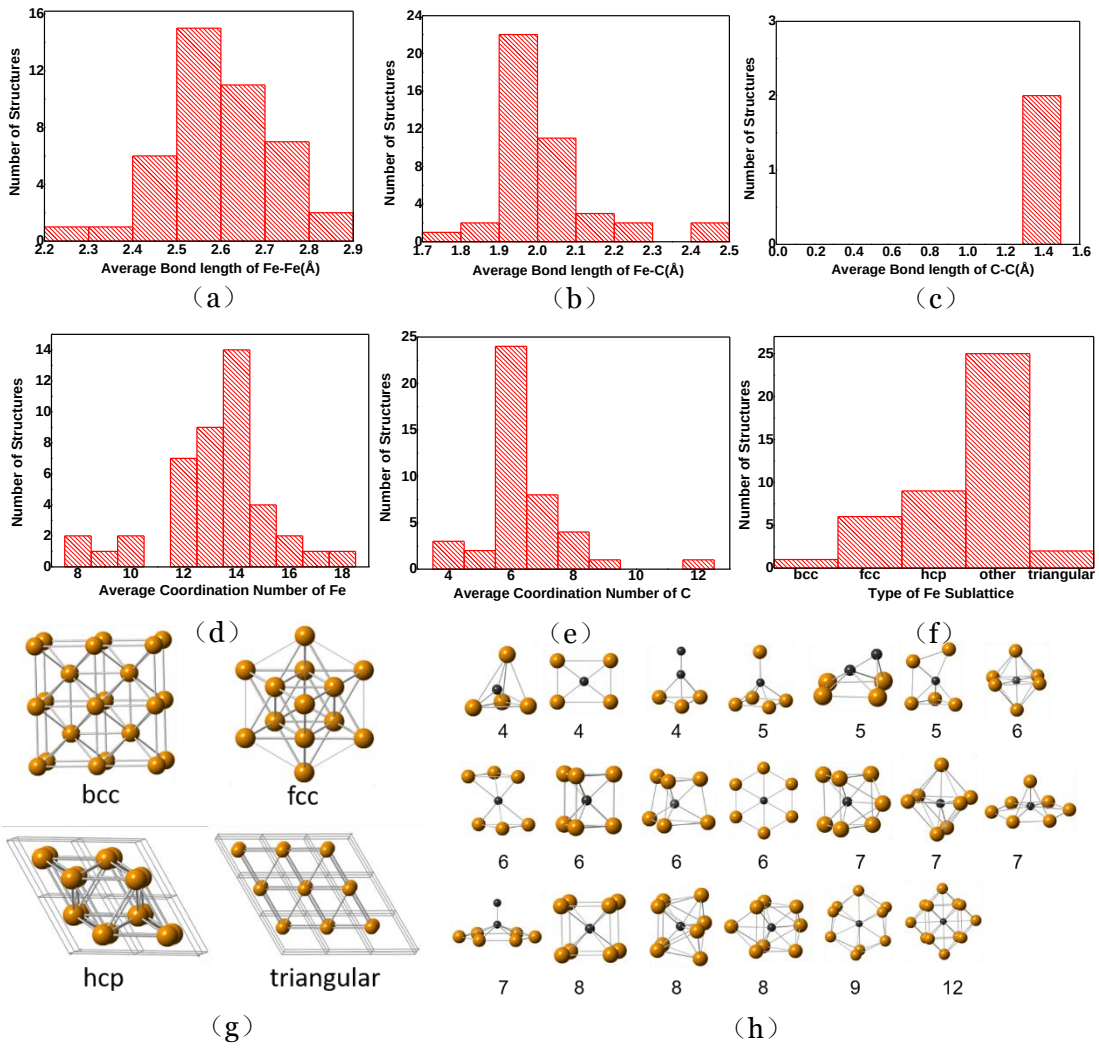
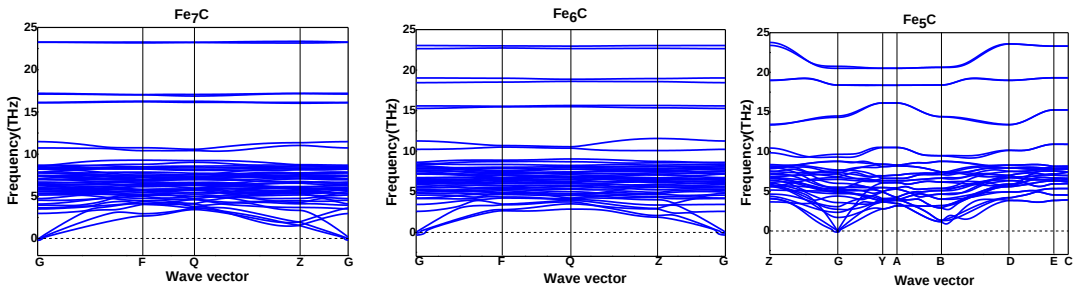
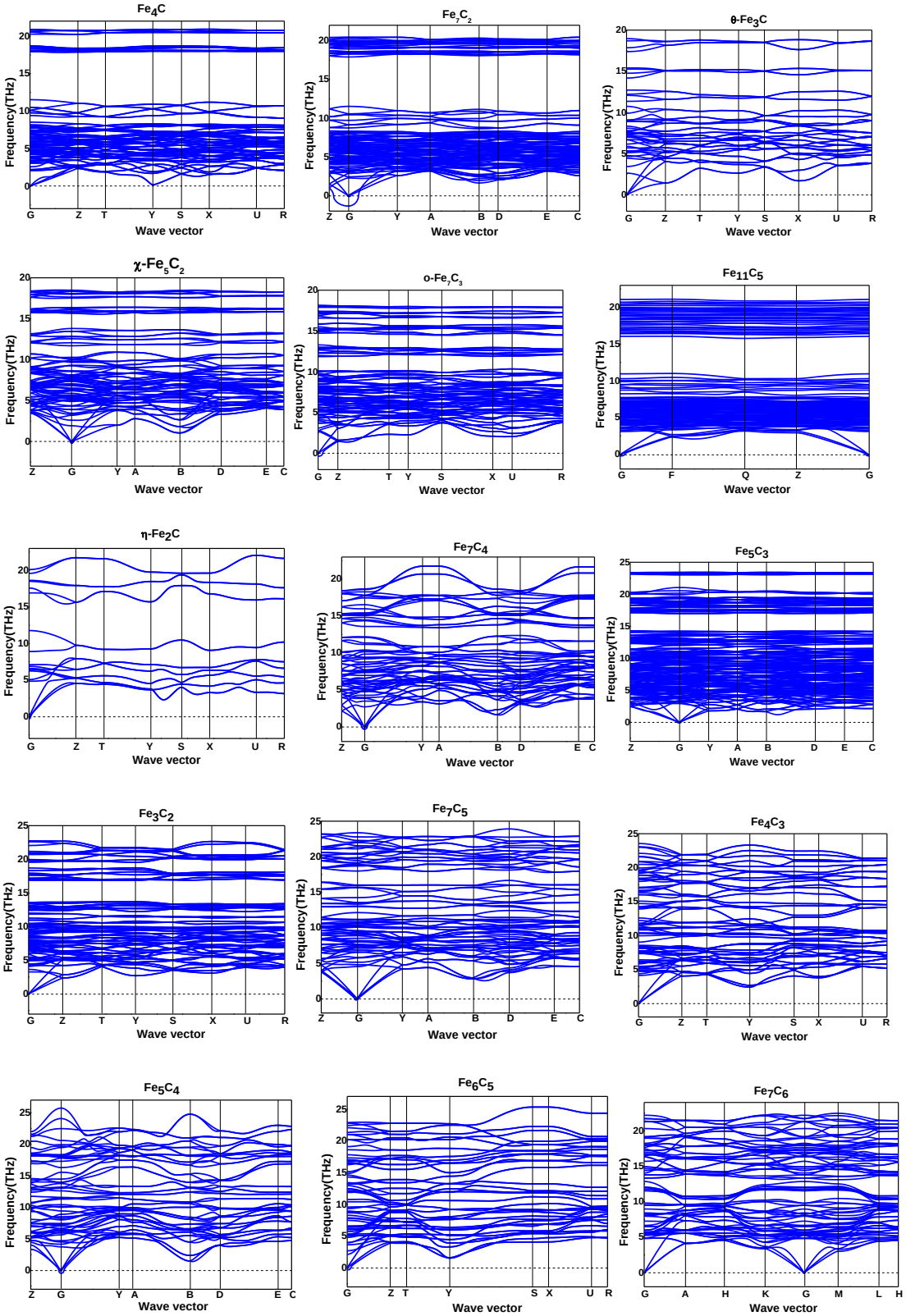


Figure S2. Structural analysis of iron carbides in database (ICSD[13,14], AFLOWLIB[15], Material Project[16], OQMD[17,18]. It's noted that the similar structures have been removed):(a) histogram of Fe-Fe average bond length (b)histogram of Fe-C average bond length (c)histogram of C-C average bond length (d)histogram of average coordination of Fe (e)histogram of average coordination of C (f)histogram of type of Fe sublattice (g)configuration of iron sublattice (h) statistics of carbon atom coordination modes(the number below refers to the coordination number)




Fe4C
Fe7C2
θ-Fe3C
χ-Fe5C2
o-Fe7C3
Fe11C5
η-Fe2C
Fe7C4
Fe5C3
Fe3C2
Fe7C5
Fe4C3
Fe5C4
Fe6C5
Fe7C6
Frequency(THz)
Wave vector

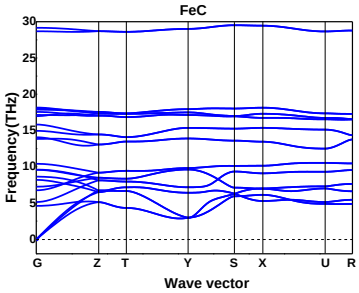
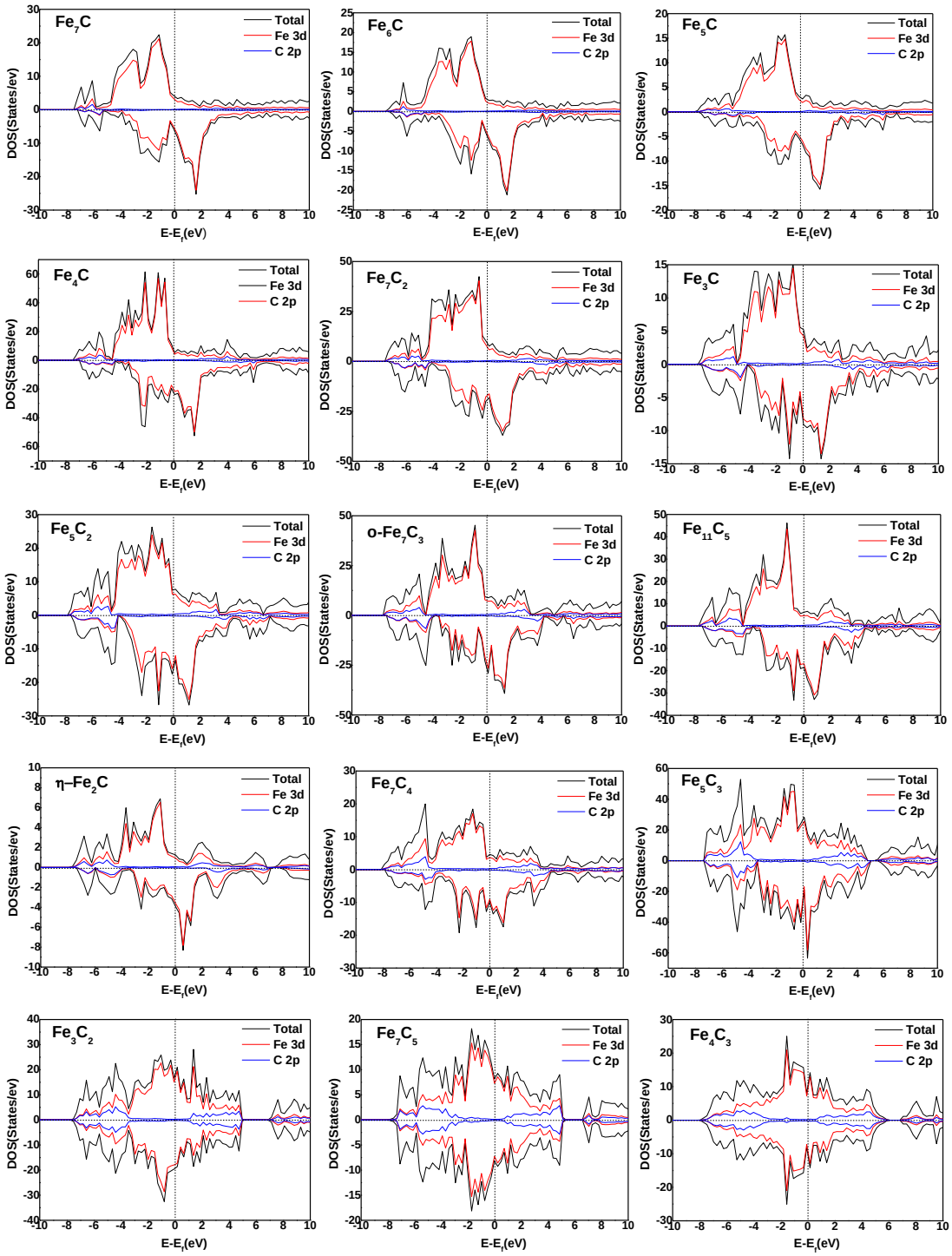


Figure S3. Phonon spectrum of the predicted iron carbides



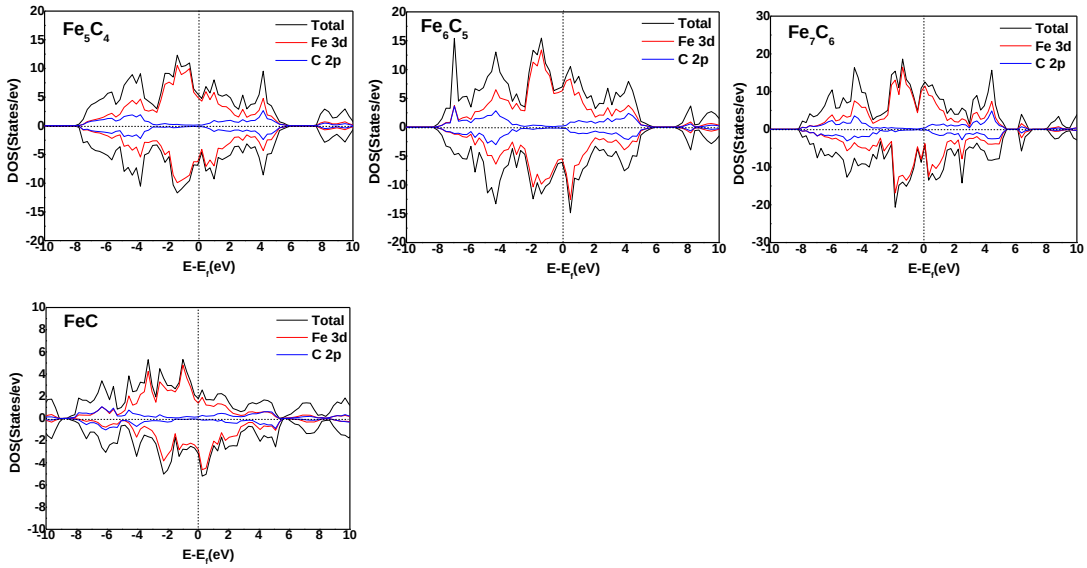


Figure S4. Partial and total densities of states of the predicted iron carbides

(Actually, the lowest valence band is almost symmetric and has no contribution to magnetic moment. Therefore, the partial density of states of C 2s is not shown in the Figure S4)

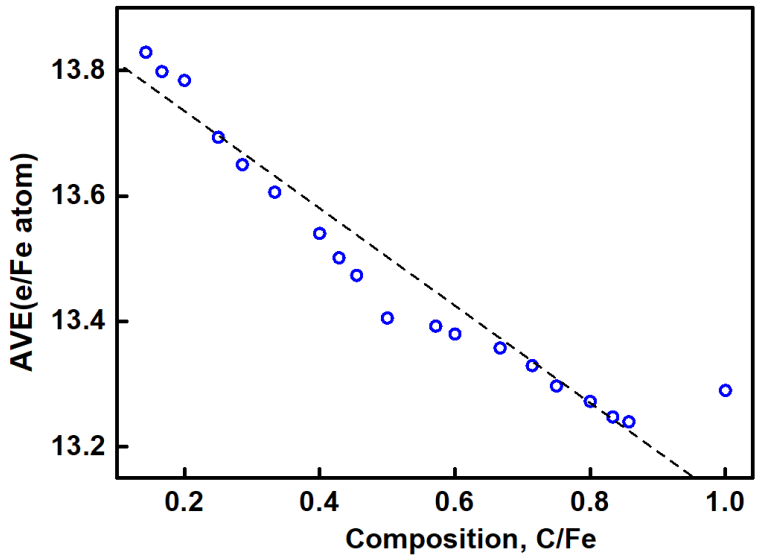


Figure S5. Average valence electrons (AVE) of iron atoms for the predicted iron carbides

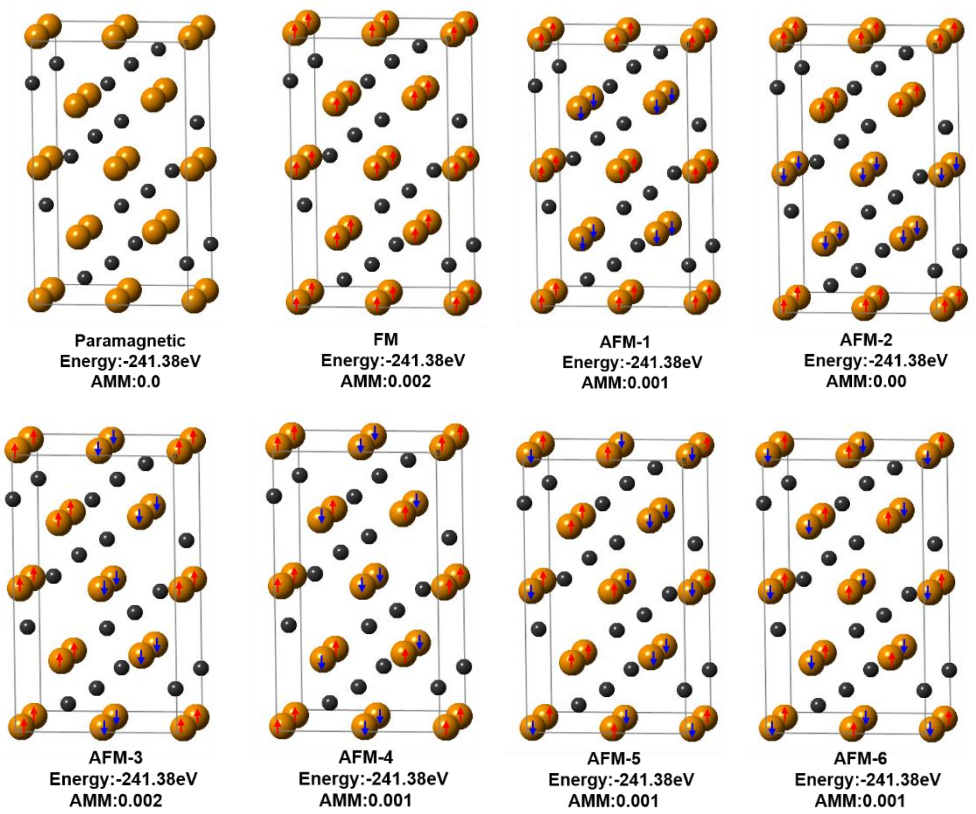
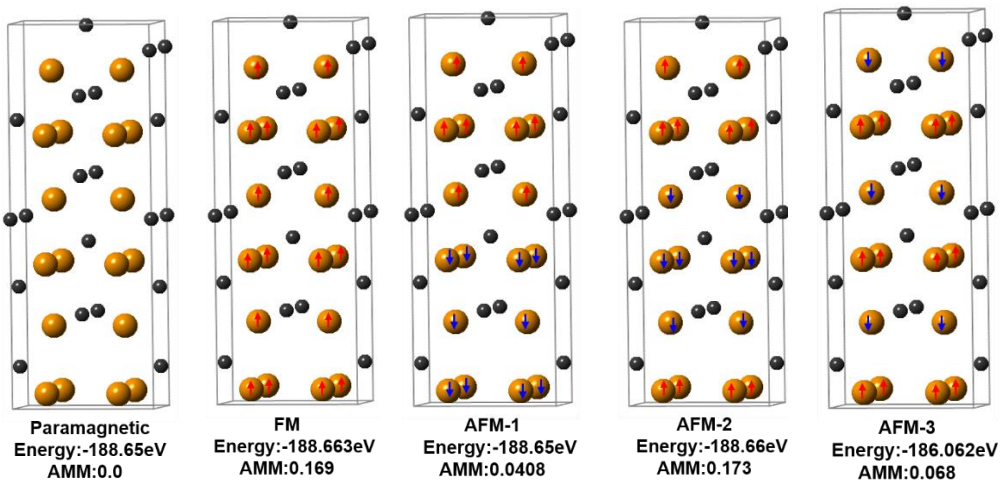


Figure S6. (a) Influence of different magnetic configurations on magnetic moments for Fe_4C_3 (FM: ferromagnetic, AFM: antiferromagnetic, Energy is the total energy of the corresponding configuration, AMM is the average magnetic moment of iron atom, unit: μ_B. The initial magnetic moments of iron and carbon were set to 3 μ_B and 0 μ_B respectively. The direction was set in the direction indicated by the arrow in the figure)



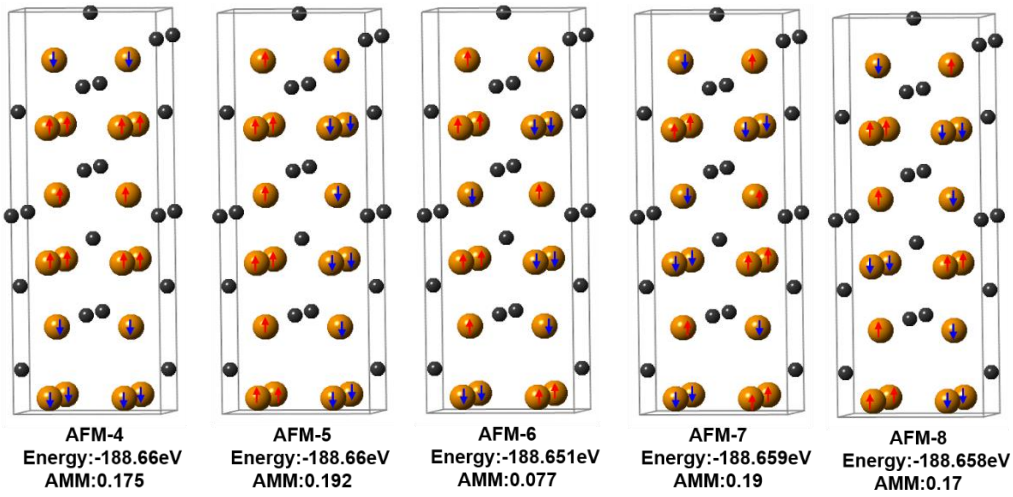


Figure S6. (b) Influence of different magnetic configurations on magnetic moments for Fe_6C_5 (The symbol description is the same as Figure S6 (a))

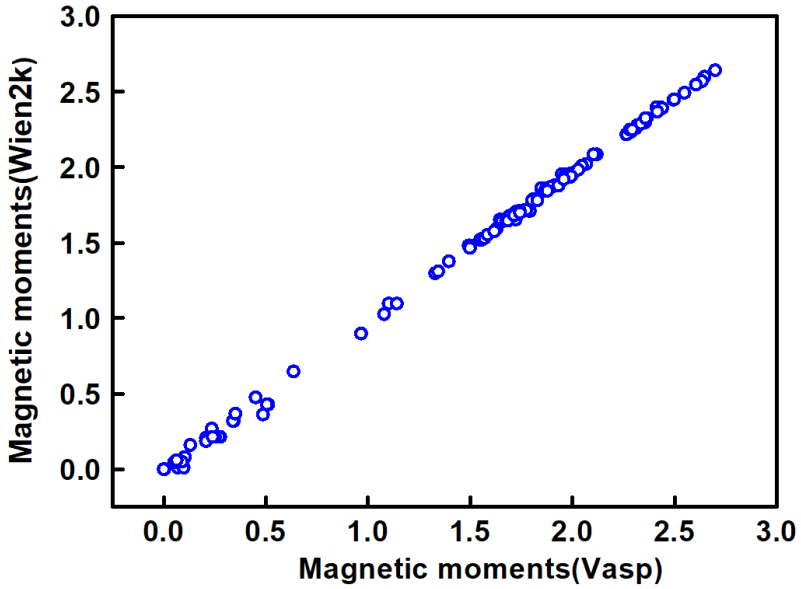
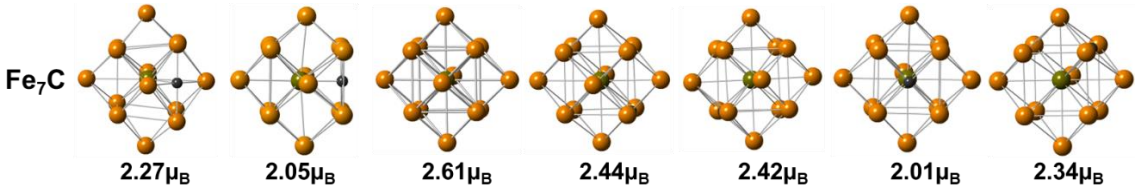
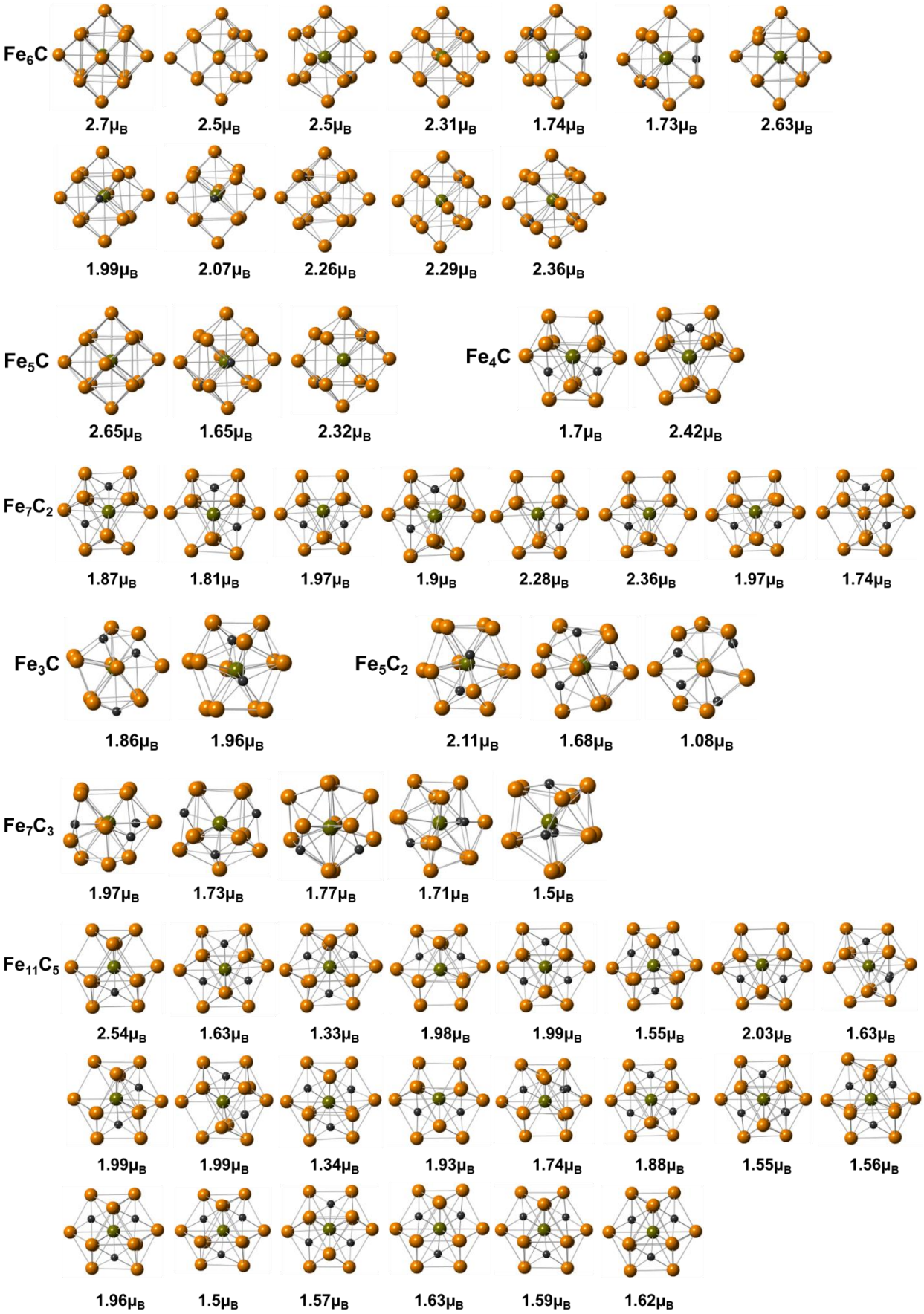


Figure S7. Correlation between magnetic moments calculated by VASP and ones calculated by WIEN2k




Fe6C
2.7μB
2.5μB
2.5μB
2.31μB
1.74μB
1.73μB
2.63μB
1.99μB
2.07μB
2.26μB
2.29μB
2.36μB
Fe5C
2.65μB
1.65μB
2.32μB
Fe4C
1.7μB
2.42μB
Fe7C2
1.87μB
1.81μB
1.97μB
1.9μB
2.28μB
2.36μB
1.97μB
1.74μB
Fe3C
1.86μB
1.96μB
Fe5C2
2.11μB
1.68μB
1.08μB
Fe7C3
1.97μB
1.73μB
1.77μB
1.71μB
1.5μB
Fe11C5
2.54μB
1.63μB
1.33μB
1.98μB
1.99μB
1.55μB
2.03μB
1.63μB
1.99μB
1.99μB
1.34μB
1.93μB
1.74μB
1.88μB
1.55μB
1.56μB
1.96μB
1.5μB
1.57μB
1.63μB
1.59μB
1.62μB

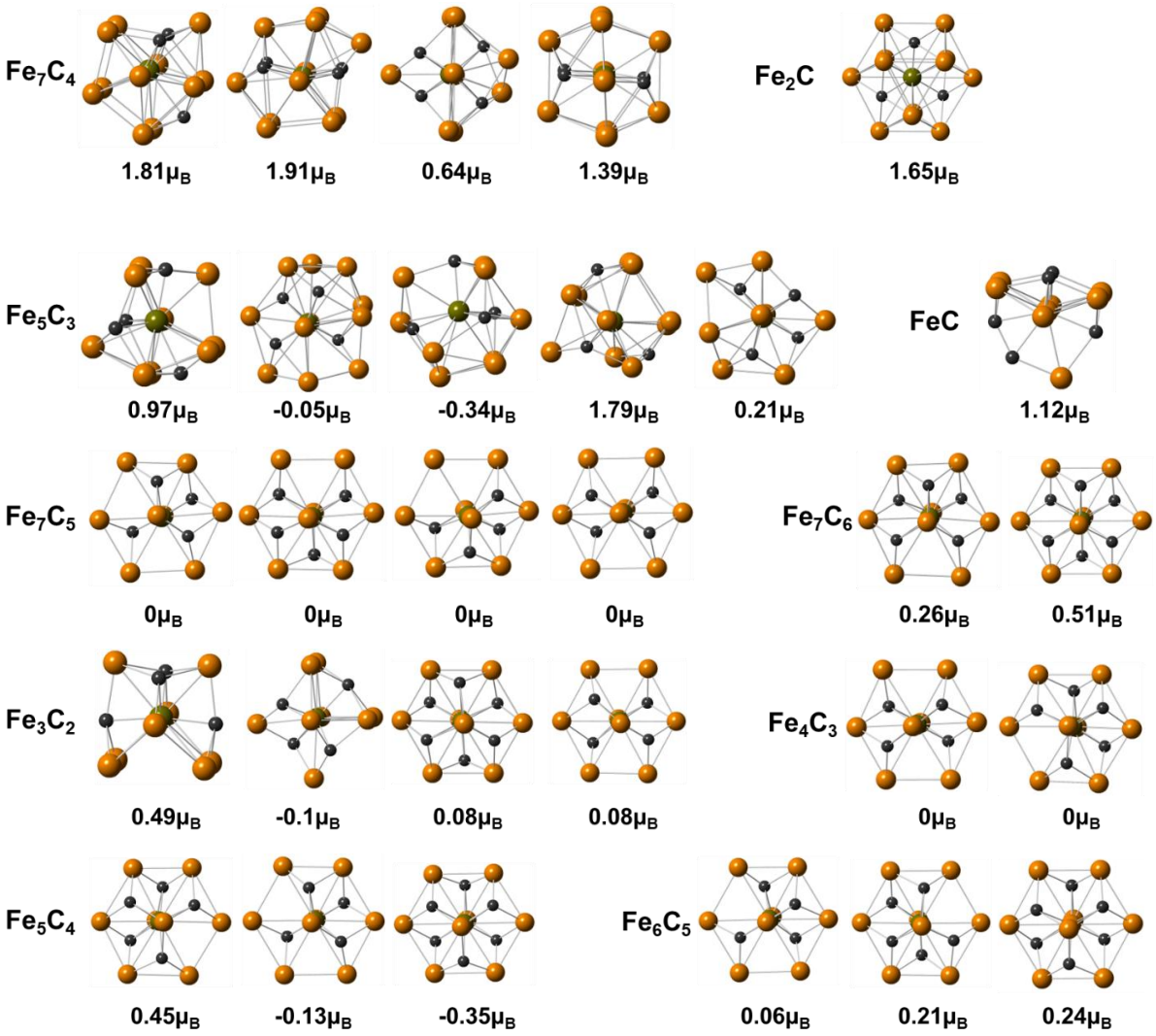


Figure S8. Local coordination configuration and central atomic magnetic moment of different iron sites of the predicted iron carbides (olive ball represents the central iron atom, orange ball represents the iron atom, black ball represents carbon atom)

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