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Supporting information for article:

First-principles investigation of V-doping effects on Fe3Cr4C3 carbide in hypereutectic Fe–Cr–C hardfacing coating

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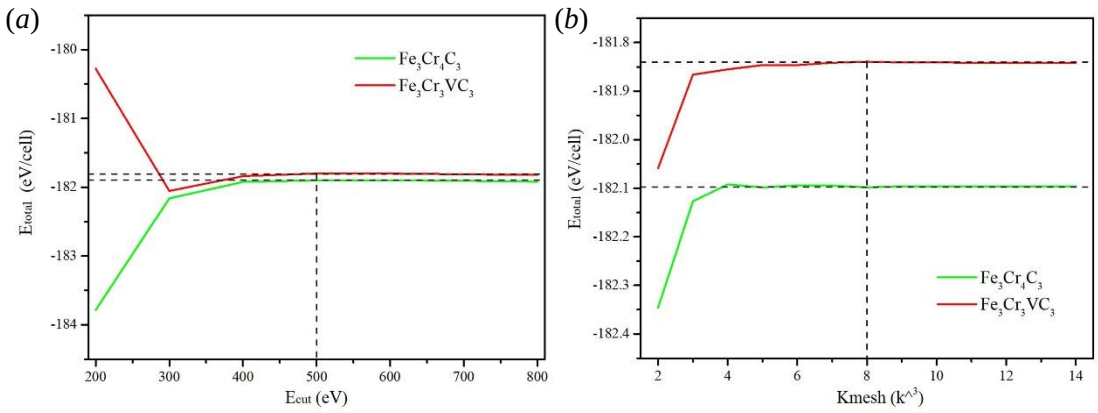

Figure S1

Convergence tests of (*a*) cutoff energy and (*b*) Kpoints.

Table S1

Structural energies of $Fe_3Cr_4C_3$ supercells with different cell sizes.

Supercell	Number of Atoms	Total energy (eV/cell)	Energy per atom (eV/atom)
1×1×1	20	-181.9049	-9.0952
1×1×2	40	-363.7897	-9.0947
2×1×1	40	-363.7901	-9.0948
2×2×1	80	-727.5819	-9.0948
2×2×2	160	-1455.1699	-9.0948

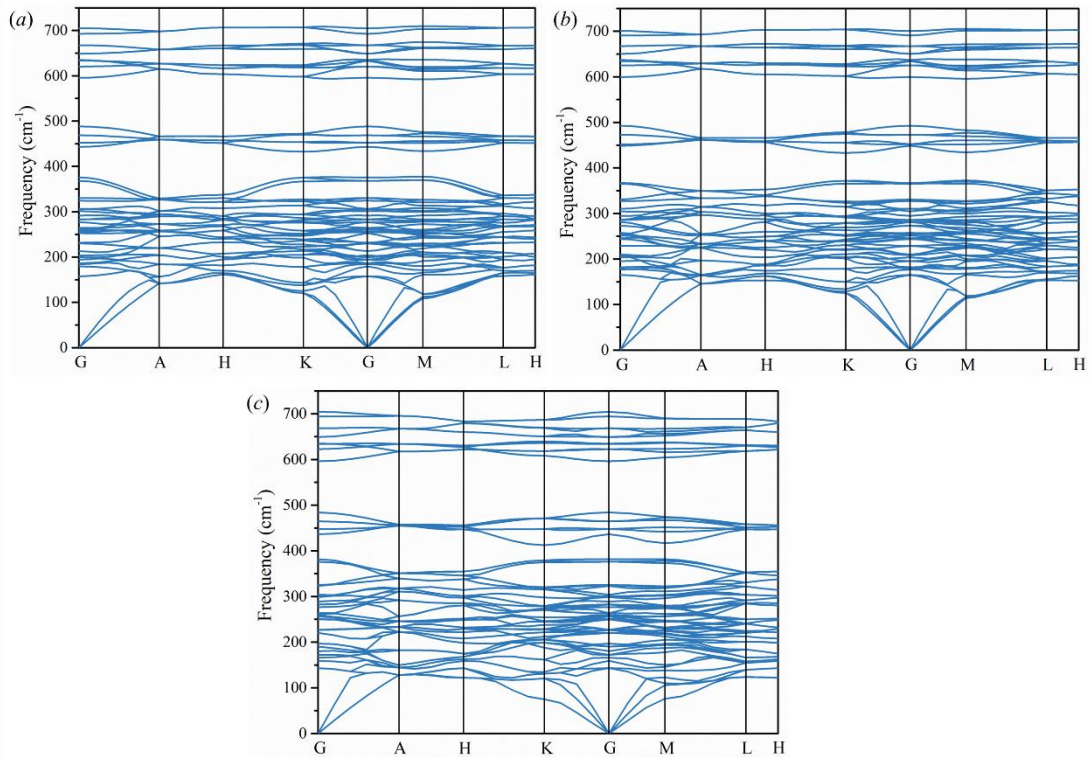

Figure S2

Phonon dispersion spectrums of (*a*) 1×1×1, (*b*) 1×1×2 and (*c*) 2×2×2 $Fe_3Cr_4C_3$ supercells.

Figure S2 shows phonon dispersion spectrums of different size $Fe_3Cr_4C_3$ supercells. No imaginary frequency appears in these spectrums, which indicates that the effect of cell size on stability can be ignored. Nevertheless, with the increase of supercell size, the interatomic forces can be calculated with increasing precision. In Figure S2(*a*), the acoustic branches of the low frequency part (0 to 150 cm^{-1}) of the phonon spectrum are densely gathered. In Figure S2(*b*), spacing between these acoustic branches is increased, which is further improved in Figure S2(*c*). Therefore, supercell size will affect the analysis of acoustic and thermodynamic properties. From the calculations of different cell sizes, the 2×2×2 supercell is large enough for accurate calculations.

Table S2

Atomic coordinates of the Fe, Cr and C atoms in $Fe_3Cr_4C_3$.

Atom type	Symmetric multiplicity	Wyckoff sites	Fractional coordinates		
			X-axis	Y-axis	Z-axis
Cr	2	b	0.3333	0.6667	0.818
Fe	6	c	0.4563	0.5437	0.318
Cr	6	c	0.1219	0.8781	0.5
C	6	c	0.1870	0.8130	0.58

All atomic coordinates in $Fe_3Cr_4C_3$ can be obtained by the symmetry operations.

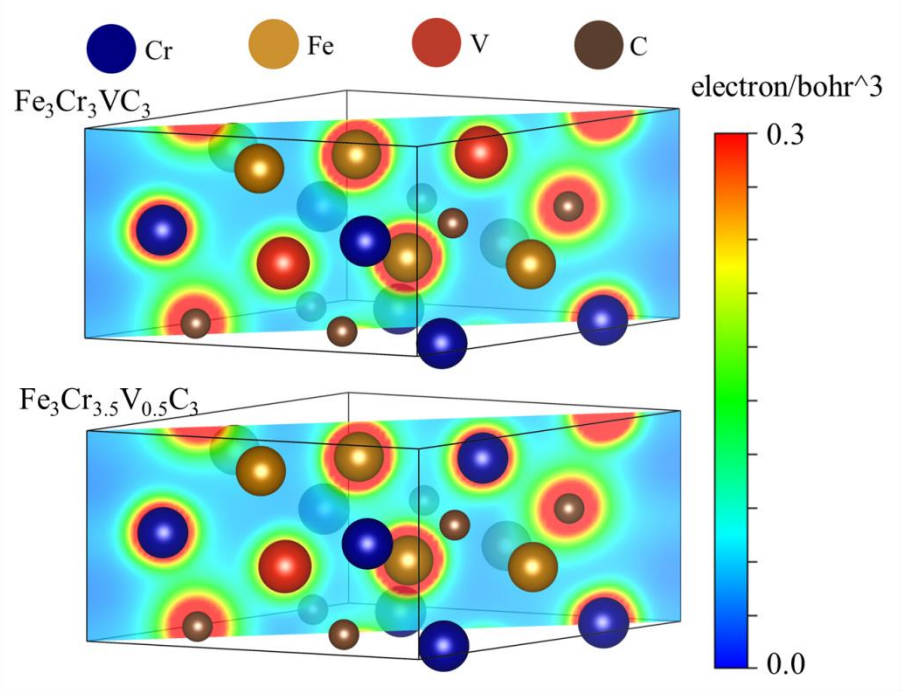

Figure S3

Charge density of (110) planes in $Fe_3Cr_3VC_3$ and $Fe_3Cr_{3.5}V_{0.5}C_3$.

Table S3

Tensile ideal strength and critical strain of $Fe_3Cr_4C_3$ and $Fe_3Cr_3VC_3$ carbides.

	$Fe_3Cr_4C_3$		$Fe_3Cr_3VC_3$	
	Ideal strength (GPa)	Critical strain (%)	Ideal strength (GPa)	Critical strain (%)
<0001>	44.42	36	48.46	31
$<2\bar{1}\bar{1}0>$	25.74	7	20.61	7
$<11\bar{2}0>$	26.47	7	20.24	7
$<11\bar{2}1>$	28.99	30	34.19	29

Table S4

Bond length in (0001) plane of $Fe_3Cr_4C_3$ with 0% strain.

Atom1	Atom2	Bond length (Å)				
C	Cr	1.99	2.02	2.04		
C	Fe	2.03	2.43			
Cr	Fe	2.50	2.54	2.55	2.67	2.76
Fe	Fe	2.45	2.50			
Cr	Cr	2.53	2.62	2.64		

Table S5

Bond length in (0001) plane of $Fe_3Cr_4C_3$ with 10% strain.

Atom1	Atom2	Bond length (Å)				
C	Cr	1.98	1.99	2.02		
C	Fe	1.94				
Cr	Fe	2.41	2.47	2.65	2.74	2.98
Fe	Fe	2.48	2.61			
Cr	Cr	2.51	2.52	2.83		

Table S6

Bond length in (0001) plane of $Fe_3Cr_4C_3$ with 20% strain.

Atom1	Atom2	Bond length (Å)			
C	Cr	1.96	1.99	2.04	
C	Fe	1.95			
Cr	Fe	2.39	2.41	2.59	3.05
Fe	Fe	2.45	2.84		
Cr	Cr	2.47	2.52	3.03	3.04

Table S7

Bond length in (0001) plane of $Fe_3Cr_4C_3$ with 36% strain.

Atom1	Atom2	Bond length (Å)
C	Cr	1.88 1.89 1.90 1.92 1.96 1.97 1.98 2.01 2.02 2.06 2.07 2.10 2.11
C	Fe	1.86 1.90 1.92 1.94 1.95 1.96 1.98 1.99 2.04 2.05 2.14 2.28
		2.32 2.34 2.36 2.37 2.38 2.39 2.40 2.42 2.472.49 2.50 2.51
Cr	Fe	2.52 2.54 2.55 2.56 2.58 2.59 2.62 2.68 2.69
		2.75 2.94 3.03 3.07 2.43 2.48 2.56 2.57 2.59 2.82
Fe	Fe	2.27 2.34 2.38 2.43 2.48 2.56 2.57 2.59 2.82
Cr	Cr	2.15 2.37 2.38 2.49 2.56 2.57 2.58 2.59 2.63 2.65 2.67 2.68
		2.69 2.72 2.81 2.95 2.99 3.02 3.11

Table S8

Bond length in $(2\bar{1}\bar{1}0)$, $(11\bar{2}0)$ and $(11\bar{2}1)$ planes of $Fe_3Cr_4C_3$ with 0% strain.

Atom1	Atom2	Bond length (Å)				
C	Cr	2.02	2.06	2.45		
C	Fe	1.91				
Cr	Fe	2.51	2.53	2.58	2.60	2.71
Fe	Fe	2.35	2.64			
Cr	Cr	2.62	2.64	2.69		

Table S9

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_4C_3$ with 3% strain.

Atom1	Atom2	Bond length (Å)					
C	Cr	1.99	2.01	2.04/2.05	2.07/2.08	2.27	2.32
C	Fe	1.86	1.89	1.92	2.43		
Cr	Fe	2.46	2.48	2.51/2.52	2.56	2.63/2.64	2.67
Fe	Fe	2.27	2.28	2.64	2.75		
Cr	Cr	2.54/2.55	2.59	2.62	2.65	2.69	2.83

Table S10

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_4C_3$ with 5% strain.

Atom1	Atom2	Bond length (Å)					
C	Cr	1.99	2.03/2.04/2.05/2.06	2.11	2.13	2.22	2.27
C	Fe	1.86	1.90	1.94	2.37	1.95	
Cr	Fe	2.42	2.47/2.49/2.50/2.51	2.56/2.57	2.62	2.65/2.66	2.73
Fe	Fe	2.25	2.26	2.65	2.81		
Cr	Cr	2.52/2.53	2.61	2.65	2.68	2.70	2.99

Table S11

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_4C_3$ with 7% strain.

Atom1	Atom2	Bond length (Å)					
C	Cr	2.00/2.01/2.02/2.03	2.06	2.15	2.17	2.21	2.40
C	Fe	1.94	1.96	1.99	2.00		
Cr	Fe	2.35/2.36/2.37	2.45/2.46	2.49/2.51	2.70	2.73	2.78
Fe	Fe	2.35	2.38	2.47	2.53		
Cr	Cr	2.45	2.49	2.61	2.65/2.66/2.67		2.80

Table S12

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_4C_3$ with 10% strain.

Atom 1	Atom 2	Bond length (Å)									
C	Cr	1.94/1.95			2.01/2.02/2.03/2.04/2.05/2.06						2.14
C	Fe	1.88/1.89		1.92		1.94/1.95			2.21	2.30	2.39
Cr	Fe	2.39	2.42	2.47-2.52		2.55-2.59	2.67	2.80-2.82		2.97	3.03
Fe	Fe		2.47		2.48		2.50		2.52		2.61
Cr	Cr	2.47	2.51	2.53	2.54	2.60	2.67	2.69	2.73	2.86	2.90

Table S13

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_4C_3$ with 20% strain.

Atom 1	Atom 2	Bond length (Å)									
C	Cr	1.88	1.93	1.97	2.03	2.07	2.08	2.09	2.12	2.13	2.17
C	Fe	1.90	1.91	1.95	1.98	2.00	2.07	2.11	2.26		
Cr	Fe	2.30	2.33 2.34	2.38	2.40	2.54- 2.56	2.59 2.60	2.65	2.71	2.82	2.95 2.96
Fe	Fe	2.47		2.54		2.56		2.62		2.70	
Cr	Cr	2.27	2.39	2.41	2.45	2.54	2.55	2.57	2.67	2.83	2.93

Table S14

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_4C_3$ with 30% strain.

Atom 1	Atom 2	Bond length (Å)										
C	Cr	1.92	1.93	1.95	1.96	2.01	2.03	2.04	2.09	2.10	2.15	
C	Fe	1.84	1.86	1.89	1.91	1.94	2.06					
Cr	Fe	2.22	2.38	2.41	2.49	2.55	2.58-2.68	2.73	2.84-2.91	2.95	3.04-3.06	3.12
Fe	Fe	2.39		2.54		2.59	2.74		2.76		2.78	
Cr	Cr	2.28	2.31 2.32	2.35 2.36	2.50	2.52	2.57	2.62 2.63	2.65	2.93 2.94	2.97	2.99

Table S15

Bond length in (0001) plane of $Fe_3Cr_3VC_3$ with 0% strain.

Atom1	Atom2	Bond length (Å)		
C	Cr	1.99	2.02	
C	Fe	2.03	2.43	
Cr	Fe	2.55	2.67	
Fe	Fe	2.45	2.50	
Cr	Cr	2.53	2.64	
C	V	2.04		
V	Fe	2.50	2.54	2.76
Cr	V	2.62		

Table S16

Bond length in (0001) plane of $Fe_3Cr_3VC_3$ with 10% strain.

Atom1	Atom2	Bond length (Å)		
C	Cr	1.99	2.04	
C	Fe	1.94		
Cr	Fe	2.49	2.76	
Fe	Fe	2.48	2.62	
Cr	Cr	2.53	2.83	
C	V	2.06		
V	Fe	2.42	2.74	2.89
Cr	V	2.50		

Table S17

Bond length in (0001) plane of $Fe_3Cr_3VC_3$ with 20% strain.

Atom1	Atom2	Bond length (Å)			
C	Cr	2.00	2.04	2.05	
C	Fe	1.94			
Cr	Fe	2.42	3.11		
Fe	Fe	2.47	2.84		
Cr	Cr	2.44	2.45	3.02	3.03
C	V	2.01			
V	Fe	2.43	2.62		
Cr	V	2.54			

Table S18

Bond length in (0001) plane of $Fe_3Cr_3VC_3$ with 30% strain.

Atom1	Atom2	Bond length (Å)									
C	Cr	1.84	1.87	1.94	1.95	1.98 -2.05	2.08	2.10	2.17		
C	Fe	1.87	1.93-2.00		2.06	2.07	2.13	2.22	2.27		
Cr	Fe	2.27	2.35 - 2.37	2.40 - 2.45	2.47 - 2.48	2.53 - 2.59	2.62 - 2.66	2.74	2.78	2.81	2.98
Fe	Fe	2.34	2.35	2.38	2.39	2.41	2.42	2.49	2.77	2.95	
Cr	Cr	2.25	2.31	2.41	2.51	2.55	2.62	2.68	2.71	2.78	3.12
C	V	1.93	2.03		2.07		2.08		2.15		
V	Fe	2.29	2.35	2.45	2.48	2.51	2.52	2.61	2.82	2.83	2.93	3.05
Cr	V	2.42	2.43	2.52	2.56	2.58	2.61	2.81	3.02	3.03	

Table S19

Bond length in $(2\bar{1}\bar{1}0)$, $(11\bar{2}0)$ and $(11\bar{2}1)$ planes of $Fe_3Cr_3VC_3$ with 0% strain.

Atom1	Atom2	Bond length (Å)		
C	Cr	2.02	2.06	2.45
C	Fe	1.91		
Cr	Fe	2.58	2.60	
Fe	Fe	2.35	2.64	
Cr	Cr	2.64	2.70	
C	V	2.06		
V	Fe	2.51	2.53	2.71
Cr	V	2.62		

Table S20

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_3VC_3$ with 3% strain.

Atom1	Atom2	Bond length (Å)					
C	Cr	1.99	2.00	2.03	2.05	2.29	2.33
C	Fe	1.87	1.89	1.92	2.46		
Cr	Fe	2.52	2.53	2.54	2.58	2.65	2.66
Fe	Fe	2.30	2.32	2.59	2.69		
Cr	Cr	2.57	2.60	2.63	2.70	2.82	
C	V	2.13	2.15				
V	Fe	2.50	2.53	2.55	2.56	2.59	
Cr	V	2.53	2.62				

Table S21

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_3VC_3$ with 5% strain.

Atom1	Atom2	Bond length (Å)						
C	Cr	1.99	2.01	2.03	2.05	2.08	2.25	2.30
C	Fe	1.87	1.89	1.94	2.43			
Cr	Fe	2.52	2.59	2.68	2.71			
Fe	Fe	2.29	2.33	2.59	2.74			
Cr	Cr	2.56	2.65	2.70	2.90			
C	V	2.14	2.17					
V	Fe	2.47	2.53	2.54	2.57	2.59		
Cr	V	2.52	2.65					

Table S22

Bond length in $(2\bar{1}\bar{1}0)$ and $(11\bar{2}0)$ planes of $Fe_3Cr_3VC_3$ with 7% strain.

Atom1	Atom2	Bond length (Å)					
C	Cr	1.20	2.03	2.04	2.09	2.22	2.25
C	Fe	1.88	1.90	1.97	2.34		
Cr	Fe	2.47	2.48	2.51	2.58	2.70	2.81
Fe	Fe	2.29	2.35	2.58	2.75		
Cr	Cr	2.54	2.61	2.68	2.70	3.06	
C	V	2.16	2.18				
V	Fe	2.40	2.52	2.56	2.58	2.59	2.62
Cr	V	2.54	2.65				

Table S23

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_3VC_3$ with 10% strain.

Atom1	Atom2	Bond length (Å)									
C	Cr	1.97	1.98	2.00	2.05	2.08	2.09	2.10	2.38	2.39	
C	Fe	1.85	1.89	1.92	1.94	1.97	2.37	2.43	2.46		
Cr	Fe	2.46	2.47	2.50 - 2.52	2.59	2.61	2.65	2.68	2.70	2.72	2.86
Fe	Fe	2.38	2.57	2.59	2.77						
Cr	Cr	2.47	2.53	2.60	2.64	2.71	2.83	2.84			
C	V	2.07	2.12	2.24							
V	Fe	2.45	2.46	2.49	2.51	2.64	2.76	2.89			
Cr	V	2.51	2.58	2.72							

Table S24

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_3VC_3$ with 20% strain.

Atom1	Atom2	Bond length (Å)									
C	Cr	1.92	1.99	2.00	2.05	2.08	2.10	2.15	2.17	2.18	
C	Fe	1.86	1.89	1.92	1.96	2.06	2.07	2.08	2.18	2.35	
Cr	Fe	2.36	2.41	2.43	2.47	2.54	2.58	2.68	2.76	2.85	2.98
Fe	Fe	2.44	2.50	2.53	2.55	2.59	3.01				
Cr	Cr	2.25	2.36	2.40	2.61	2.64	2.77	2.78	3.07		
C	V	1.99	2.17	2.35							
V	Fe	2.30	2.34	2.42	2.53	2.54	2.68	2.76			
Cr	V	2.46	2.69	2.75	2.76						

Table S25

Bond length in $(11\bar{2}1)$ plane of $Fe_3Cr_3VC_3$ with 29% strain.

Atom1	Atom2	Bond length (Å)							
C	Cr	1.91	1.96	1.98	2.15				
C	Fe	1.88	1.89	1.96	1.97	1.98	2.00	2.02	2.12
Cr	Fe	2.48/ 2.49	2.55/ 2.56	2.59/ 2.60	2.67	2.73/ 2.74	2.85	2.91	2.95
Fe	Fe	2.51	2.55	2.62	2.67				
Cr	Cr	2.18	2.42/ 2.43	2.47	2.53	2.78	2.91/ 2.92	3.05	
C	V	1.99	2.21	2.39					
V	Fe	2.17	2.27	2.49	2.60	2.76	2.77		
Cr	V	2.41	2.75	2.89					