Supplementary information:

Table 1a. On site magnetic moments of TM doping in Type 1 finite SiNT's.

TM-atoms	**n=1 (in μ_B)**		**n=2 (in μ_B)**		**n=3 (in μ_B)**		**n=4 (in μ_B)**	
	Cr_nSi_{12n}	$Cr_{2n-1}Si_{12n}$	Cr_nSi_{12n}	$Cr_{2n-1}Si_{12n}$	Cr_nSi_{12n}	$Cr_{2n-1}Si_{12n}$	Cr_nSi_{12n}	$Cr_{2n-1}Si_{12n}$
1st	0	0	2.141	1.227	-1.712	0	-1.596	0
2nd			2.230	-0.125	2.493	0	2.794	0
3rd				1.337	1.505	0	2.970	0
4th						0	-2.053	0
5th						0		0
6th								0
7th								0
Total	**0**	**0**	**6**	**4**	**2**	**0**	**2**	**0**
	Mn_nSi_{12n}	$Mn_{2n-1}Si_{12n}$	Mn_nSi_{12n}	$Mn_{2n-1}Si_{12n}$	Mn_nSi_{12n}	$Mn_{2n-1}Si_{12n}$	Mn_nSi_{12n}	$Mn_{2n-1}Si_{12n}$
1st	1.526	1.526	-2.301	0.477	-1.898	-2.662	-1.733	0.102
2nd			-2.302	-2.350	2.436	-0.275	-1.989	2.413
3rd				-1.148	-1.868	-2.101	-2.097	2.582
4th						-1.499	-1.663	-0.030
5th						-2.026		1.852
6th								2.146
7th								2.363
Total	**1**	**1**	**6**	**3**	**1**	**9**	**8**	**13**
	Fe_nSi_{12n}	$Fe_{2n-1}Si_{12n}$	Fe_nSi_{12n}	$Fe_{2n-1}Si_{12n}$	Fe_nSi_{12n}	$Fe_{2n-1}Si_{12n}$	Fe_nSi_{12n}	$Fe_{2n-1}Si_{12n}$
1st	0	0	-1.733	-1.480	0.963	-2.125	1.222	-1.457
2nd			-1.717	-1.499	-1.293	-1.458	-1.138	-2.016
3rd				-2.586	0.921	-1.507	-1.132	-1.994
4th						-1.922	1.220	-1.479
5th						-1.971		-2.016
6th								-2.138
7th								-2.061
Total	**0**	**0**	**4**	**6**	**0**	**8**	**2**	**12**

Table 1b: On site Magnetic moment of Type 1 finite sized clusters and functionalized cluster assemblies

Magnetization at $Si_{12}Cr$ cluster

Atoms	s	p	d	Total
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Cr	0.000	0.000	0.000	0.000
Total	0.000	-0.000	0.000	0.000

Magnetization at $Si_{12}Mn$ cluster

Atoms	s	p	d	Total
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Si	-0.001	-0.018	0.000	-0.019
Mn	0.015	0.016	1.495	1.526
Total	0.001	-0.202	1.495	1.294

Magnetization at $Si_{12}Fe$ cluster

Atoms	s	p	d	Total
Si	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Fe	-0.000	-0.000	-0.000	-0.000
Total	-0.000	0.000	-0.000	-0.000

Magnetization at $Si_{24}Cr_3$ cluster

Atoms	s	p	d	Total
Si	0.001	0.005	0.000	0.006
Si	0.003	-0.005	0.000	-0.003
Si	0.002	0.008	0.000	0.010
Si	-0.001	0.008	0.000	0.007
Si	0.001	-0.018	0.000	-0.017
Si	0.004	-0.010	0.000	-0.006
Si	0.008	0.035	0.000	0.043
Si	0.005	0.030	0.000	0.034
Si	0.005	0.011	0.000	0.016
Si	0.004	0.011	0.000	0.015
Si	0.002	0.010	0.000	0.011
Si	0.004	0.017	0.000	0.021
Si	0.014	0.013	0.000	0.027
Si	0.001	0.006	0.000	0.006
Si	0.003	0.005	0.000	0.009
Si	0.015	0.024	0.000	0.040
Si	0.003	0.018	0.000	0.022
Si	-0.000	-0.000	0.000	-0.000
Si	0.002	-0.007	0.000	-0.005
Si	-0.002	-0.003	0.000	-0.005
Si	0.003	0.014	0.000	0.017
Si	0.003	-0.002	0.000	0.001
Si	-0.000	0.008	0.000	0.007
Si	-0.001	0.006	0.000	0.005
Cr	0.014	0.012	1.200	1.657
Cr	0.015	0.018	1.304	1.767
Cr	0.000	0.007	-0.133	-0.125
Total	0.108	0.222	2.371	3.561

Magnetization at $Si_{24}Mn_3$ cluster

Atoms	s	p	d	Total
Si	-0.003	-0.023	0.000	-0.026
Si	-0.002	-0.020	0.000	-0.023
Si	-0.002	-0.020	0.000	-0.022
Si	-0.002	-0.020	0.000	-0.022
Si	-0.002	-0.022	0.000	-0.024
Si	-0.003	-0.024	0.000	-0.027
Si	-0.000	-0.009	0.000	-0.009
Si	0.002	-0.005	0.000	-0.004
Si	0.002	-0.005	0.000	-0.003
Si	0.001	-0.006	0.000	-0.005
Si	0.001	-0.006	0.000	-0.005
Si	-0.001	-0.009	0.000	-0.009
Si	0.002	0.008	0.000	0.011
Si	0.003	0.009	0.000	0.012
Si	0.002	-0.003	0.000	-0.001
Si	0.002	0.002	0.000	0.004
Si	0.004	0.005	0.000	0.009
Si	0.003	0.001	0.000	0.004
Si	0.003	0.034	0.000	0.037
Si	0.004	0.037	0.000	0.041
Si	0.003	0.031	0.000	0.034
Si	0.003	0.032	0.000	0.035
Si	0.004	0.040	0.000	0.045
Si	0.004	0.040	0.000	0.043
Mn	0.006	0.008	0.463	0.477
Mn	-0.022	-0.025	-2.304	-2.350
Mn	-0.008	-0.005	-1.135	-1.148
Total	0.004	0.045	-2.976	-2.927

Magnetization at $Si_{24}Fe_3$ cluster

Atoms	s	p	d	Total
Si	0.002	-0.007	0.000	-0.004
Si	0.002	-0.005	0.000	-0.003
Si	0.002	-0.005	0.000	-0.003
Si	0.002	-0.005	0.000	-0.003
Si	0.002	-0.007	0.000	-0.004
Si	0.002	-0.006	0.000	-0.004
Si	-0.003	-0.011	0.000	-0.014
Si	-0.003	-0.009	0.000	-0.011
Si	-0.003	-0.009	0.000	-0.012
Si	-0.003	-0.009	0.000	-0.011
Si	-0.003	-0.010	0.000	-0.013
Si	-0.003	-0.010	0.000	-0.013
Si	-0.003	-0.009	0.000	-0.012
Si	-0.003	-0.010	0.000	-0.013
Si	-0.003	-0.010	0.000	-0.013
Si	-0.003	-0.010	0.000	-0.013
Si	-0.003	-0.009	0.000	-0.012
Si	-0.003	-0.009	0.000	-0.012
Si	0.002	-0.006	0.000	-0.003
Si	0.002	-0.006	0.000	-0.004
Si	0.002	-0.007	0.000	-0.004
Si	0.002	-0.007	0.000	-0.005
Si	0.002	-0.005	0.000	-0.003
Si	0.002	-0.006	0.000	-0.003
Fe	-0.011	-0.009	-1.460	-1.480
Fe	-0.011	-0.009	-1.479	-1.499
Fe	-0.016	-0.006	-2.565	-2.586
Total	-0.048	-0.207	-5.504	-5.758

Magnetization at $Si_{36}Cr_5$ cluster

Atoms	s	p	d	Total
Si	0.000	0.000	0.000	0.000

Magnetization at $Si_{36}Mn_5$ cluster

Atoms	s	p	d	Total
Si	0.001	0.010	0.000	0.010

Magnetization at $Si_{36}Fe_5$ cluster

Atoms	s	p	d	Total
Si	0.002	0.005	0.000	0.007

Si	0.000	0.000	0.000	0.000	Si	0.000	-0.007	0.000	-0.006	Si	0.001	0.008	0.000	0.009
Si	0.000	0.000	0.000	0.000	Si	0.000	-0.015	0.000	-0.015	Si	-0.000	0.003	0.000	0.003
Si	0.000	0.000	0.000	0.000	Si	-0.003	-0.005	0.000	-0.008	Si	0.001	0.007	0.000	0.008
Si	0.000	0.000	0.000	0.000	Si	0.002	-0.005	0.000	-0.003	Si	0.002	0.015	0.000	0.017
Si	0.000	0.000	0.000	0.000	Si	0.003	-0.002	0.000	0.001	Si	0.002	0.010	0.000	0.012
Si	0.000	0.000	0.000	0.000	Si	-0.003	-0.021	0.000	-0.024	Si	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000	Si	0.002	-0.001	0.000	0.001	Si	0.002	0.012	0.000	0.014
Si	0.000	0.000	0.000	0.000	Si	0.003	0.014	0.000	0.017	Si	0.003	0.009	0.000	0.012
Si	0.000	0.000	0.000	0.000	Si	-0.001	-0.009	0.000	-0.010	Si	0.001	0.008	0.000	0.009
Si	0.000	0.000	0.000	0.000	Si	0.000	0.003	0.000	0.003	Si	0.002	0.015	0.000	0.017
Si	0.000	0.000	0.000	0.000	Si	0.001	0.007	0.000	0.008	Si	0.000	0.009	0.000	0.009
Si	-0.000	-0.000	0.000	-0.000	Si	-0.005	-0.004	0.000	-0.008	Si	-0.007	-0.002	0.000	-0.009
Si	-0.000	-0.000	0.000	-0.000	Si	-0.000	-0.004	0.000	-0.004	Si	0.000	0.006	0.000	0.006
Si	-0.000	-0.000	0.000	-0.000	Si	-0.000	-0.006	0.000	-0.007	Si	-0.003	0.004	0.000	0.001
Si	-0.000	-0.000	0.000	-0.000	Si	-0.005	-0.007	0.000	-0.012	Si	0.001	0.008	0.000	0.008
Si	-0.000	-0.000	0.000	-0.000	Si	0.000	-0.008	0.000	-0.008	Si	-0.002	0.004	0.000	0.001
Si	-0.000	-0.000	0.000	-0.000	Si	-0.002	-0.007	0.000	-0.009	Si	-0.002	0.001	0.000	-0.001
Si	-0.000	-0.000	0.000	-0.000	Si	0.001	0.007	0.000	0.008	Si	0.001	0.018	0.000	0.019
Si	-0.000	-0.000	0.000	-0.000	Si	-0.002	0.001	0.000	-0.002	Si	0.003	0.013	0.000	0.016
Si	-0.000	-0.000	0.000	-0.000	Si	0.002	0.001	0.000	0.003	Si	0.002	0.012	0.000	0.015
Si	-0.000	-0.000	0.000	-0.000	Si	0.002	-0.000	0.000	0.001	Si	0.003	0.008	0.000	0.011
Si	-0.000	-0.000	0.000	-0.000	Si	-0.001	0.005	0.000	0.004	Si	0.003	0.023	0.000	0.026
Si	-0.000	-0.000	0.000	-0.000	Si	0.001	0.008	0.000	0.009	Si	0.003	0.015	0.000	0.017
Si	-0.000	-0.000	0.000	-0.000	Si	-0.004	-0.013	0.000	-0.017	Si	-0.001	0.008	0.000	0.007
Si	-0.000	-0.000	0.000	-0.000	Si	-0.003	0.007	0.000	0.004	Si	0.001	0.010	0.000	0.010
Si	-0.000	-0.000	0.000	-0.000	Si	-0.006	0.009	0.000	0.003	Si	-0.006	0.004	0.000	-0.002
Si	-0.000	-0.000	0.000	-0.000	Si	-0.004	-0.018	0.000	-0.022	Si	-0.001	0.006	0.000	0.005
Si	-0.000	-0.000	0.000	-0.000	Si	0.001	0.004	0.000	0.005	Si	-0.001	0.009	0.000	0.007
Si	-0.000	-0.000	0.000	-0.000	Si	0.000	0.012	0.000	0.012	Si	0.000	0.009	0.000	0.009
Si	-0.000	-0.000	0.000	-0.000	Si	0.001	0.029	0.000	0.030	Si	0.004	0.025	0.000	0.028
Si	-0.000	-0.000	0.000	-0.000	Si	0.004	0.018	0.000	0.022	Si	0.003	0.007	0.000	0.010
Si	-0.000	-0.000	0.000	-0.000	Si	0.002	0.024	0.000	0.027	Si	0.001	0.017	0.000	0.018
Si	-0.000	-0.000	0.000	-0.000	Si	0.003	0.030	0.000	0.033	Si	0.003	0.014	0.000	0.017
Si	-0.000	-0.000	0.000	-0.000	Si	0.002	0.016	0.000	0.019	Si	0.002	0.018	0.000	0.020
Si	-0.000	-0.000	0.000	-0.000	Si	0.002	0.027	0.000	0.028	Si	0.003	0.015	0.000	0.019
Cr	-0.000	-0.000	-0.001	-0.001	Mn	-0.019	-0.034	-2.608	-2.662	Fe	-0.016	-0.027	-2.082	-2.125
Cr	0.000	0.000	0.000	0.000	Mn	-0.000	0.006	-0.281	-0.275	Fe	-0.010	-0.017	-1.431	-1.458
Cr	0.000	0.000	0.000	0.000	Mn	-0.017	-0.022	-2.062	-2.101	Fe	-0.011	-0.015	-1.481	-1.507
Cr	0.000	0.000	0.000	0.000	Mn	-0.008	-0.011	-1.480	-1.499	Fe	-0.009	-0.005	-1.908	-1.922
Cr	0.000	0.000	0.000	0.000	Mn	-0.012	-0.011	-2.003	-2.026	Fe	-0.010	-0.004	-1.957	-1.971
Total	-0.000	0.000	-0.000	-0.000	Total	-0.062	0.026	-8.434	-8.470	Total	-0.032	0.280	-8.859	-8.610

Table 1c: On site Magnetic moment for Type 2 finite sized clusters and functionalized cluster assemblies

Magnetization of $Si_{16}Cr$					Magnetization of $Si_{16}Mn$					Magnetization of $Si_{16}Fe$				
Atoms	s	p	d	Total	Atoms	s	p	d	Total	Atoms	s	p	d	Total
Si	0.000	-0.000	0.000	-0.000	Si	0.000	0.015	0.000	0.016	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.016	0.000	-0.017	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.000	-0.015	0.000	-0.016	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.000	-0.019	0.000	-0.019	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	0.002	0.009	0.000	0.011	Si	0.000	0.000	0.000	0.000
Si	0.000	-0.000	0.000	-0.000	Si	0.020	0.098	0.000	0.118	Si	0.000	0.000	0.000	0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.012	0.000	-0.013	Si	0.000	0.000	0.000	0.000

Si	0.000	-0.000	0.000	-0.000	Si	-0.001	0.000	0.000	-0.000	Si	0.000	0.000	0.000	0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.003	0.000	-0.005	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.003	-0.004	0.000	-0.006	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	0.002	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.020	0.000	-0.022	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.020	0.000	-0.022	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.001	0.000	-0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.003	-0.018	0.000	-0.021	Si	0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000	Si	-0.003	-0.026	0.000	-0.029	Si	0.000	-0.000	0.000	-0.000
Cr	0.000	0.000	0.000	0.000	Mn	0.011	0.014	1.052	1.077	Fe	0.000	0.000	0.000	0.000
Total	0.000	-0.000	0.000	0.000	Total	0.013	-0.015	1.052	1.051	Total	0.000	-0.000	0.000	0.000
Magnetization of $Si_{28}Cr_2$					Magnetization of $Si_{28}Mn_2$					Magnetization of $Si_{28}Fe_2$				
Atoms	s	p	d	Total	Atoms	s	p	d	Total	Atoms	s	p	d	Total
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.016	0.000	-0.017	Si	0.003	0.002	0.000	0.005
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.014	0.000	-0.016	Si	0.001	0.003	0.000	0.004
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.014	0.000	-0.016	Si	-0.000	0.004	0.000	0.004
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.015	0.000	-0.016	Si	-0.000	0.001	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	0.007	-0.014	0.000	-0.007	Si	0.003	-0.001	0.000	0.002
Si	0.000	-0.000	0.000	-0.000	Si	0.008	-0.010	0.000	-0.003	Si	0.005	0.006	0.000	0.011
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.014	0.000	-0.015	Si	0.000	0.001	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.001	0.000	-0.001	Si	0.002	0.008	0.000	0.010
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.001	0.000	-0.001	Si	-0.000	0.001	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	-0.004	-0.013	0.000	-0.016	Si	0.003	-0.015	0.000	-0.011
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.009	0.000	-0.012	Si	0.004	-0.008	0.000	-0.003
Si	0.000	-0.000	0.000	-0.000	Si	-0.004	-0.013	0.000	-0.017	Si	0.009	-0.008	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.010	0.000	-0.012	Si	0.002	-0.009	0.000	-0.007
Si	0.000	-0.000	0.000	-0.000	Si	0.007	-0.001	0.000	0.006	Si	-0.003	-0.000	0.000	-0.003
Si	0.000	-0.000	0.000	-0.000	Si	0.006	-0.003	0.000	0.003	Si	-0.000	0.010	0.000	0.009
Si	0.000	-0.000	0.000	-0.000	Si	0.007	-0.001	0.000	0.005	Si	0.012	0.074	0.000	0.086
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.010	0.000	-0.012	Si	0.004	-0.007	0.000	-0.003
Si	0.000	-0.000	0.000	-0.000	Si	-0.004	-0.013	0.000	-0.016	Si	0.009	-0.008	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	0.006	-0.003	0.000	0.003	Si	-0.000	0.010	0.000	0.010
Si	0.000	-0.000	0.000	-0.000	Si	-0.004	-0.012	0.000	-0.016	Si	0.004	-0.015	0.000	-0.011
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.010	0.000	-0.012	Si	0.003	-0.001	0.000	0.003
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.001	0.000	-0.001	Si	-0.000	0.001	0.000	0.001
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.001	0.000	-0.001	Si	0.003	0.008	0.000	0.010
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.014	0.000	-0.016	Si	0.001	0.003	0.000	0.004
Si	0.000	-0.000	0.000	-0.000	Si	-0.001	-0.016	0.000	-0.018	Si	0.003	0.002	0.000	0.005
Si	0.000	-0.000	0.000	-0.000	Si	0.007	-0.013	0.000	-0.007	Si	0.002	-0.000	0.000	0.002
Si	0.000	-0.000	0.000	-0.000	Si	0.007	-0.010	0.000	-0.003	Si	0.005	0.006	0.000	0.011
Si	0.000	-0.000	0.000	-0.000	Si	-0.002	-0.014	0.000	-0.016	Si	-0.000	0.004	0.000	0.004
Cr	0.000	0.000	0.000	0.000	Mn	0.009	0.012	0.903	0.925	Fe	0.001	0.002	0.042	0.046
Cr	0.000	0.000	0.000	0.000	Mn	0.004	0.006	0.466	0.476	Fe	0.010	0.018	1.110	1.138
Total	0.000	-0.000	0.000	0.000	Total	0.031	-0.248	1.369	1.152	Total	0.085	0.093	1.152	1.331
Magnetization of $Si_{40}Cr_3$					Magnetization of $Si_{40}Mn_3$					Magnetization of $Si_{40}Fe_3$				
Atoms	s	p	d	Total	Atoms	s	p	d	Total	Atoms	s	p	d	Total
Si	0.008	0.009	0.000	0.017	Si	0.010	0.011	0.000	0.022	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.013	0.000	0.014	Si	0.002	-0.001	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.013	0.000	0.014	Si	0.004	-0.003	0.000	0.002	Si	0.000	-0.000	0.000	-0.000
Si	0.008	0.009	0.000	0.017	Si	0.011	0.011	0.000	0.022	Si	0.000	-0.000	0.000	-0.000
Si	-0.000	0.016	0.000	0.016	Si	0.003	0.017	0.000	0.021	Si	0.000	-0.000	0.000	-0.000
Si	-0.000	0.016	0.000	0.016	Si	0.003	0.017	0.000	0.020	Si	0.000	-0.000	0.000	-0.000

Si	0.008	0.008	0.000	0.017	Si	0.011	0.010	0.000	0.020	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.006	-0.005	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.000	0.000	0.001	Si	0.004	-0.009	0.000	-0.006	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.006	-0.005	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.004	-0.010	0.000	-0.006	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.013	0.000	0.015	Si	0.003	-0.005	0.000	-0.002	Si	0.000	-0.000	0.000	-0.000
Si	0.008	0.009	0.000	0.017	Si	0.010	0.010	0.000	0.020	Si	0.000	-0.000	0.000	-0.000
Si	-0.000	0.016	0.000	0.016	Si	0.003	0.016	0.000	0.019	Si	0.000	-0.000	0.000	-0.000
Si	-0.000	0.016	0.000	0.016	Si	0.003	0.016	0.000	0.019	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.013	0.000	0.014	Si	0.002	-0.001	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.002	0.000	0.002	Si	0.003	-0.007	0.000	-0.003	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.001	-0.000	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.001	-0.000	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.002	0.000	0.002	Si	0.003	-0.007	0.000	-0.003	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.018	-0.011	0.000	0.007	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.018	-0.010	0.000	0.008	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.002	0.000	0.003	Si	0.003	-0.007	0.000	-0.003	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.002	0.000	0.001	Si	0.001	0.005	0.000	0.005	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.002	0.000	0.002	Si	0.000	0.005	0.000	0.005	Si	0.000	-0.000	0.000	-0.000
Si	-0.002	-0.015	0.000	-0.018	Si	0.001	-0.039	0.000	-0.037	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.003	0.000	0.002	Si	0.001	-0.014	0.000	-0.014	Si	0.000	-0.000	0.000	-0.000
Si	-0.002	-0.015	0.000	-0.018	Si	0.002	-0.039	0.000	-0.037	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.003	0.000	0.002	Si	0.001	-0.015	0.000	-0.014	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.003	0.000	0.002	Si	0.001	-0.015	0.000	-0.014	Si	0.000	-0.000	0.000	-0.000
Si	-0.002	-0.015	0.000	-0.018	Si	0.002	-0.038	0.000	-0.036	Si	0.000	-0.000	0.000	-0.000
Si	-0.002	-0.015	0.000	-0.017	Si	0.002	-0.039	0.000	-0.037	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.002	0.000	0.002	Si	0.000	-0.015	0.000	-0.014	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.002	0.000	0.002	Si	0.001	0.005	0.000	0.005	Si	0.000	-0.000	0.000	-0.000
Si	-0.001	0.002	0.000	0.002	Si	0.000	0.004	0.000	0.005	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.002	0.000	0.000	0.002	Si	0.000	-0.000	0.000	-0.000
Si	0.001	0.002	0.000	0.002	Si	0.004	-0.006	0.000	-0.002	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.018	-0.011	0.000	0.007	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.018	-0.009	0.000	0.009	Si	0.000	-0.000	0.000	-0.000
Si	0.000	0.001	0.000	0.001	Si	0.002	-0.000	0.000	0.001	Si	0.000	-0.000	0.000	-0.000
Cr	-0.001	-0.003	-0.081	-0.085	Mn	0.013	0.018	1.414	1.445	Fe	0.000	0.000	0.000	0.000
Cr	0.014	0.020	1.247	1.280	Mn	0.029	0.027	2.683	2.739	Fe	0.000	0.000	0.000	0.000
Cr	-0.002	-0.003	-0.032	-0.038	Mn	0.010	0.014	1.109	1.133	Fe	0.000	0.000	0.000	0.000
Total	0.037	0.142	1.133	1.313	Total	0.238	-0.132	5.206	5.312	Total	0.000	-0.000	0.000	0.000

Table 1d: Onsite magnetic moment of each unit cell in 1D SiNT's.

Magnetization of $Si_{24}Cr_4$: Type 1					**Magnetization of $Si_{24}Mn_4$: Type 1**					**Magnetization of $Si_{24}Fe_4$: Type 1**				
Atoms	s	p	d	Total	Atoms	s	p	d	Total	Atoms	s	p	d	Total
Si	0.000	0.014	0.000	0.014	Si	-0.002	-0.017	0.000	-0.019	Si	0.001	0.010	0.000	0.011
Si	-0.000	0.014	0.000	0.014	Si	-0.002	-0.017	0.000	-0.019	Si	0.001	0.010	0.000	0.011
Si	0.001	0.032	0.000	0.032	Si	-0.002	-0.017	0.000	-0.019	Si	0.001	0.015	0.000	0.016
Si	-0.000	0.008	0.000	0.008	Si	0.000	-0.018	0.000	-0.018	Si	-0.000	-0.003	0.000	-0.003
Si	-0.000	0.008	0.000	0.008	Si	0.000	-0.018	0.000	-0.018	Si	-0.000	-0.003	0.000	-0.003
Si	0.001	0.031	0.000	0.032	Si	-0.002	-0.017	0.000	-0.019	Si	0.001	0.015	0.000	0.016
Si	0.000	0.020	0.000	0.020	Si	0.001	-0.007	0.000	-0.007	Si	0.001	0.000	0.000	0.002
Si	0.000	0.020	0.000	0.020	Si	0.001	-0.008	0.000	-0.007	Si	0.001	0.000	0.000	0.002
Si	-0.000	0.006	0.000	0.006	Si	0.001	-0.008	0.000	-0.007	Si	0.001	-0.005	0.000	-0.004
Si	0.000	0.028	0.000	0.028	Si	-0.000	-0.003	0.000	-0.003	Si	0.002	0.016	0.000	0.017
Si	0.000	0.028	0.000	0.028	Si	-0.000	-0.002	0.000	-0.003	Si	0.002	0.016	0.000	0.017

Si	-0.001	0.005	0.000	0.005
Si	-0.000	0.008	0.000	0.008
Si	-0.000	0.008	0.000	0.008
Si	0.000	0.014	0.000	0.014
Si	0.001	0.032	0.000	0.033
Si	0.001	0.031	0.000	0.031
Si	-0.000	0.014	0.000	0.014
Si	0.000	0.028	0.000	0.028
Si	0.000	0.028	0.000	0.028
Si	0.000	0.020	0.000	0.020
Si	-0.001	0.005	0.000	0.005
Si	-0.000	0.006	0.000	0.005
Si	0.000	0.020	0.000	0.020
Cr	0.001	-0.001	0.115	0.115
Cr	0.001	-0.001	0.122	0.122
Cr	0.001	-0.001	0.119	0.320
Cr	0.001	-0.001	0.115	0.315
Total	0.005	0.426	0.471	1.302

Si	0.001	-0.007	0.000	-0.007
Si	0.000	-0.018	0.000	-0.018
Si	0.000	-0.018	0.000	-0.018
Si	-0.002	-0.017	0.000	-0.019
Si	-0.002	-0.017	0.000	-0.019
Si	-0.002	-0.017	0.000	-0.019
Si	-0.002	-0.017	0.000	-0.019
Si	-0.000	-0.003	0.000	-0.003
Si	-0.000	-0.003	0.000	-0.003
Si	0.001	-0.007	0.000	-0.007
Si	0.001	-0.007	0.000	-0.007
Si	0.001	-0.008	0.000	-0.007
Si	0.001	-0.008	0.000	-0.007
Mn	0.012	0.010	1.883	1.905
Mn	0.012	0.010	1.881	1.904
Mn	0.014	0.014	2.061	2.090
Mn	0.014	0.014	2.061	2.089
Total	0.048	-0.233	7.887	7.701

Si	0.001	-0.005	0.000	-0.004
Si	-0.000	-0.003	0.000	-0.003
Si	-0.000	-0.003	0.000	-0.003
Si	0.001	0.010	0.000	0.011
Si	0.001	0.015	0.000	0.016
Si	0.001	0.015	0.000	0.016
Si	0.001	0.010	0.000	0.011
Si	0.002	0.016	0.000	0.017
Si	0.002	0.016	0.000	0.017
Si	0.001	0.000	0.000	0.002
Si	0.001	-0.005	0.000	-0.004
Si	0.001	-0.005	0.000	-0.004
Si	0.001	0.000	0.000	0.002
Fe	0.006	0.011	1.964	1.980
Fe	0.006	0.011	1.964	1.980
Fe	0.005	0.006	1.934	1.946
Fe	0.005	0.006	1.934	1.945
Total	0.045	0.166	7.796	8.007

Magnetization of $Si_{24}Cr_2$:Type 2

Atoms	s	p	d	Total
Si	-0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	0.000	0.000	-0.000
Si	0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	0.000	0.000	0.000	0.000
Si	-0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	-0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	0.000	0.000	0.000	0.000
Si	0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Si	0.000	-0.000	0.000	-0.000
Si	-0.000	-0.000	0.000	-0.000
Si	-0.000	0.000	0.000	0.000
Si	-0.000	-0.000	0.000	-0.000
Cr	0.000	-0.000	0.000	0.000
Cr	0.000	-0.000	-0.000	-0.000
Total	-0.000	-0.000	0.000	0.000

Magnetization of $Si_{24}Mn_2$:Type 2

Atoms	s	p	d	Total
Si	0.003	0.002	0.000	0.005
Si	0.011	-0.005	0.000	0.006
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.002	0.000	0.005
Si	0.003	0.025	0.000	0.028
Si	0.003	0.025	0.000	0.028
Si	0.003	0.002	0.000	0.005
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.002	0.000	0.005
Si	0.003	0.025	0.000	0.028
Si	0.003	0.024	0.000	0.028
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.002	0.000	0.005
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.002	0.000	0.005
Si	0.011	-0.005	0.000	0.006
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.002	0.000	0.005
Si	0.003	0.002	0.000	0.005
Si	0.011	-0.005	0.000	0.006
Si	0.003	0.025	0.000	0.028
Si	0.003	0.024	0.000	0.028
Si	0.003	0.024	0.000	0.028
Si	0.003	0.025	0.000	0.028
Mn	0.024	0.026	2.425	2.675
Mn	0.024	0.026	2.429	2.679
Total	0.188	0.226	4.855	5.868

Magnetization of $Si_{24}Fe_2$:Type 2

Atoms	s	p	d	Total
Si	0.005	-0.008	0.000	-0.003
Si	0.004	0.024	0.000	0.029
Si	0.004	0.024	0.000	0.029
Si	0.005	-0.009	0.000	-0.004
Si	-0.003	-0.047	0.000	-0.050
Si	-0.003	-0.047	0.000	-0.050
Si	0.005	-0.008	0.000	-0.003
Si	0.004	0.024	0.000	0.029
Si	0.005	-0.009	0.000	-0.004
Si	-0.003	-0.046	0.000	-0.050
Si	-0.003	-0.047	0.000	-0.050
Si	0.004	0.024	0.000	0.029
Si	0.000	0.025	0.000	0.025
Si	0.003	0.001	0.000	0.004
Si	0.000	0.025	0.000	0.025
Si	0.003	0.001	0.000	0.003
Si	0.003	0.000	0.000	0.003
Si	0.000	0.025	0.000	0.025
Si	0.000	0.025	0.000	0.025
Si	0.003	0.001	0.000	0.004
Si	0.001	0.001	0.000	0.002
Si	0.001	0.001	0.000	0.002
Si	0.001	0.001	0.000	0.002
Si	0.001	0.001	0.000	0.002
Fe	-0.002	-0.006	-0.725	-0.734
Fe	-0.006	-0.009	-1.283	-1.298
Total	0.031	-0.034	-2.008	-2.012

Magnetization of $Si_{30}Cr_2$:Type 3

Atoms	s	p	d	Total
Si	-0.003	0.011	0.000	0.008

Magnetization of $Si_{30}Mn_2$:Type 3

Atoms	s	p	d	Total
Si	-0.006	-0.013	0.000	-0.019

Magnetization of $Si_{30}Fe_2$:Type 3

Atoms	s	p	d	Total
Si	0.004	-0.008	0.000	-0.004

Si	-0.001	-0.014	0.000	-0.015
Si	0.003	-0.004	0.000	-0.000
Si	0.002	-0.020	0.000	-0.018
Si	0.003	0.012	0.000	0.015
Si	0.008	0.047	0.000	0.055
Si	0.003	0.012	0.000	0.015
Si	0.007	0.047	0.000	0.054
Si	0.005	0.009	0.000	0.014
Si	0.005	0.022	0.000	0.026
Si	0.008	0.072	0.000	0.081
Si	0.002	0.011	0.000	0.013
Si	0.010	0.017	0.000	0.026
Si	-0.000	0.007	0.000	0.007
Si	-0.000	-0.009	0.000	-0.010
Si	0.004	-0.008	0.000	-0.005
Si	0.002	-0.003	0.000	-0.002
Si	0.001	-0.022	0.000	-0.021
Si	0.006	0.045	0.000	0.052
Si	0.008	0.072	0.000	0.080
Si	0.005	0.009	0.000	0.014
Si	0.010	0.017	0.000	0.027
Si	0.002	0.010	0.000	0.012
Si	-0.000	-0.006	0.000	-0.006
Si	-0.001	-0.012	0.000	-0.013
Si	0.007	0.006	0.000	0.012
Si	0.004	0.008	0.000	0.012
Si	0.007	0.006	0.000	0.013
Si	-0.000	0.011	0.000	0.011
Si	0.003	0.008	0.000	0.012
Cr	0.043	0.040	2.753	3.836
Cr	0.054	0.035	3.435	3.524
Total	0.205	0.435	6.188	7.828

Si	-0.004	-0.015	0.000	-0.019
Si	0.003	0.049	0.000	0.052
Si	0.003	0.045	0.000	0.048
Si	0.000	-0.005	0.000	-0.005
Si	0.004	0.050	0.000	0.054
Si	0.002	-0.001	0.000	0.001
Si	0.005	0.046	0.000	0.051
Si	0.005	0.021	0.000	0.026
Si	0.007	0.014	0.000	0.020
Si	0.003	0.026	0.000	0.029
Si	0.002	-0.016	0.000	-0.014
Si	0.002	0.018	0.000	0.019
Si	0.002	-0.017	0.000	-0.015
Si	-0.002	-0.020	0.000	-0.021
Si	-0.007	0.005	0.000	-0.002
Si	-0.002	-0.017	0.000	-0.020
Si	-0.003	-0.000	0.000	-0.004
Si	0.004	0.050	0.000	0.054
Si	0.005	0.044	0.000	0.049
Si	0.009	0.015	0.000	0.024
Si	0.006	0.020	0.000	0.026
Si	0.003	-0.005	0.000	-0.002
Si	-0.004	-0.020	0.000	-0.023
Si	-0.010	-0.056	0.000	-0.066
Si	0.004	0.004	0.000	0.008
Si	0.002	0.004	0.000	0.007
Si	0.002	0.014	0.000	0.017
Si	0.002	0.002	0.000	0.004
Si	0.003	0.004	0.000	0.007
Mn	0.032	0.030	3.207	3.569
Mn	0.029	0.018	3.667	3.714
Total	0.102	0.293	6.874	7.569

Si	-0.001	-0.015	0.000	-0.015
Si	0.006	0.077	0.000	0.083
Si	0.014	0.093	0.000	0.108
Si	0.004	-0.014	0.000	-0.010
Si	0.008	0.055	0.000	0.063
Si	0.000	-0.007	0.000	-0.007
Si	0.001	0.004	0.000	0.005
Si	0.003	0.026	0.000	0.029
Si	0.004	0.020	0.000	0.024
Si	0.002	0.006	0.000	0.008
Si	0.002	0.003	0.000	0.005
Si	0.006	0.023	0.000	0.030
Si	0.001	-0.017	0.000	-0.016
Si	-0.000	-0.011	0.000	-0.011
Si	0.013	0.104	0.000	0.116
Si	-0.001	-0.019	0.000	-0.020
Si	-0.002	0.001	0.000	-0.001
Si	-0.001	0.005	0.000	0.004
Si	0.007	0.039	0.000	0.046
Si	0.004	0.047	0.000	0.051
Si	0.006	0.021	0.000	0.026
Si	0.003	-0.024	0.000	-0.021
Si	0.002	-0.021	0.000	-0.019
Si	-0.001	-0.005	0.000	-0.006
Si	0.002	0.014	0.000	0.016
Si	0.001	0.015	0.000	0.016
Si	0.004	0.013	0.000	0.017
Si	0.002	0.010	0.000	0.012
Si	0.002	0.008	0.000	0.011
Fe	0.023	0.017	2.176	2.816
Fe	0.023	0.014	2.342	2.379
Total	0.141	0.474	4.518	5.732

Magnetization of $Si_{36}Cr_2$:Type 4

Atoms	s	p	d	Total
Si	0.007	0.033	0.000	0.040
Si	-0.000	-0.004	0.000	-0.004
Si	0.007	0.033	0.000	0.040
Si	0.006	0.033	0.000	0.039
Si	0.000	-0.003	0.000	-0.003
Si	0.006	0.031	0.000	0.037
Si	0.000	-0.004	0.000	-0.004
Si	0.006	0.031	0.000	0.037
Si	0.003	0.019	0.000	0.022
Si	0.003	0.020	0.000	0.023
Si	0.006	0.032	0.000	0.038
Si	0.000	-0.004	0.000	-0.003
Si	0.003	0.020	0.000	0.022
Si	0.000	-0.004	0.000	-0.003
Si	-0.000	-0.004	0.000	-0.004
Si	0.007	0.033	0.000	0.040
Si	-0.000	-0.004	0.000	-0.004
Si	0.007	0.034	0.000	0.040
Si	0.006	0.032	0.000	0.038
Si	0.006	0.032	0.000	0.038

Magnetization of $Si_{36}Mn_2$:Type 4

Atoms	s	p	d	Total
Si	0.003	0.025	0.000	0.029
Si	0.000	-0.002	0.000	-0.002
Si	0.003	0.025	0.000	0.028
Si	0.003	0.025	0.000	0.028
Si	-0.000	-0.002	0.000	-0.003
Si	0.003	0.025	0.000	0.028
Si	-0.000	-0.002	0.000	-0.002
Si	0.005	0.032	0.000	0.037
Si	0.002	0.023	0.000	0.025
Si	0.001	0.021	0.000	0.022
Si	0.003	0.025	0.000	0.028
Si	-0.000	-0.002	0.000	-0.002
Si	0.001	0.021	0.000	0.022
Si	0.000	-0.002	0.000	-0.002
Si	-0.000	-0.002	0.000	-0.002
Si	0.003	0.025	0.000	0.028
Si	0.000	-0.002	0.000	-0.002
Si	0.005	0.034	0.000	0.039
Si	0.005	0.034	0.000	0.039
Si	0.003	0.025	0.000	0.029

Magnetization of $Si_{36}Fe_2$:Type 4

Atoms	s	p	d	Total
Si	-0.005	-0.029	0.000	-0.034
Si	-0.001	-0.018	0.000	-0.019
Si	-0.002	-0.012	0.000	-0.014
Si	-0.001	-0.008	0.000	-0.009
Si	0.000	0.006	0.000	0.006
Si	0.000	0.003	0.000	0.003
Si	0.002	0.009	0.000	0.011
Si	0.000	0.003	0.000	0.003
Si	-0.000	0.003	0.000	0.002
Si	-0.000	0.003	0.000	0.002
Si	0.000	0.005	0.000	0.006
Si	-0.000	-0.001	0.000	-0.001
Si	0.001	0.007	0.000	0.008
Si	0.000	0.006	0.000	0.006
Si	0.000	-0.008	0.000	-0.008
Si	-0.005	-0.029	0.000	-0.034
Si	-0.003	-0.022	0.000	-0.025
Si	-0.002	-0.012	0.000	-0.014
Si	0.003	0.012	0.000	0.016
Si	0.004	0.012	0.000	0.016

Si	0.003	0.019	0.000	0.022	Si	0.002	0.023	0.000	0.025	Si	-0.001	0.008	0.000	0.007
Si	0.003	0.020	0.000	0.022	Si	0.001	0.021	0.000	0.022	Si	-0.001	0.008	0.000	0.007
Si	0.000	-0.004	0.000	-0.003	Si	-0.000	-0.002	0.000	-0.003	Si	0.003	0.018	0.000	0.021
Si	-0.000	-0.004	0.000	-0.004	Si	-0.000	-0.002	0.000	-0.003	Si	-0.004	-0.053	0.000	-0.058
Si	-0.000	-0.004	0.000	-0.004	Si	-0.000	-0.002	0.000	-0.003	Si	-0.003	-0.022	0.000	-0.025
Si	-0.000	0.002	0.000	0.002	Si	0.002	0.007	0.000	0.009	Si	0.000	0.006	0.000	0.006
Si	-0.000	0.002	0.000	0.002	Si	0.002	0.010	0.000	0.011	Si	0.001	-0.000	0.000	0.000
Si	-0.000	0.002	0.000	0.002	Si	0.001	0.010	0.000	0.011	Si	0.003	0.013	0.000	0.016
Si	-0.000	0.002	0.000	0.002	Si	0.002	0.007	0.000	0.009	Si	0.003	0.013	0.000	0.016
Si	-0.000	0.002	0.000	0.002	Si	0.001	0.010	0.000	0.011	Si	0.002	-0.001	0.000	0.001
Si	0.003	0.019	0.000	0.022	Si	0.001	0.021	0.000	0.022	Si	0.001	0.007	0.000	0.008
Si	-0.000	0.002	0.000	0.002	Si	0.002	0.010	0.000	0.011	Si	0.000	0.006	0.000	0.006
Si	-0.000	-0.004	0.000	-0.004	Si	-0.000	-0.002	0.000	-0.002	Si	-0.001	-0.018	0.000	-0.018
Si	0.006	0.033	0.000	0.039	Si	0.005	0.032	0.000	0.037	Si	-0.001	-0.008	0.000	-0.009
Si	0.000	-0.004	0.000	-0.003	Si	0.000	-0.002	0.000	-0.002	Si	-0.000	-0.001	0.000	-0.001
Si	0.006	0.032	0.000	0.038	Si	0.003	0.026	0.000	0.029	Si	0.001	0.005	0.000	0.006
Cr	0.060	0.050	3.715	3.926	Mn	0.049	0.031	3.629	3.709	Fe	0.014	0.015	1.806	1.935
Cr	0.051	0.049	3.693	3.893	Mn	0.049	0.031	3.627	3.707	Fe	0.019	0.010	2.235	2.164
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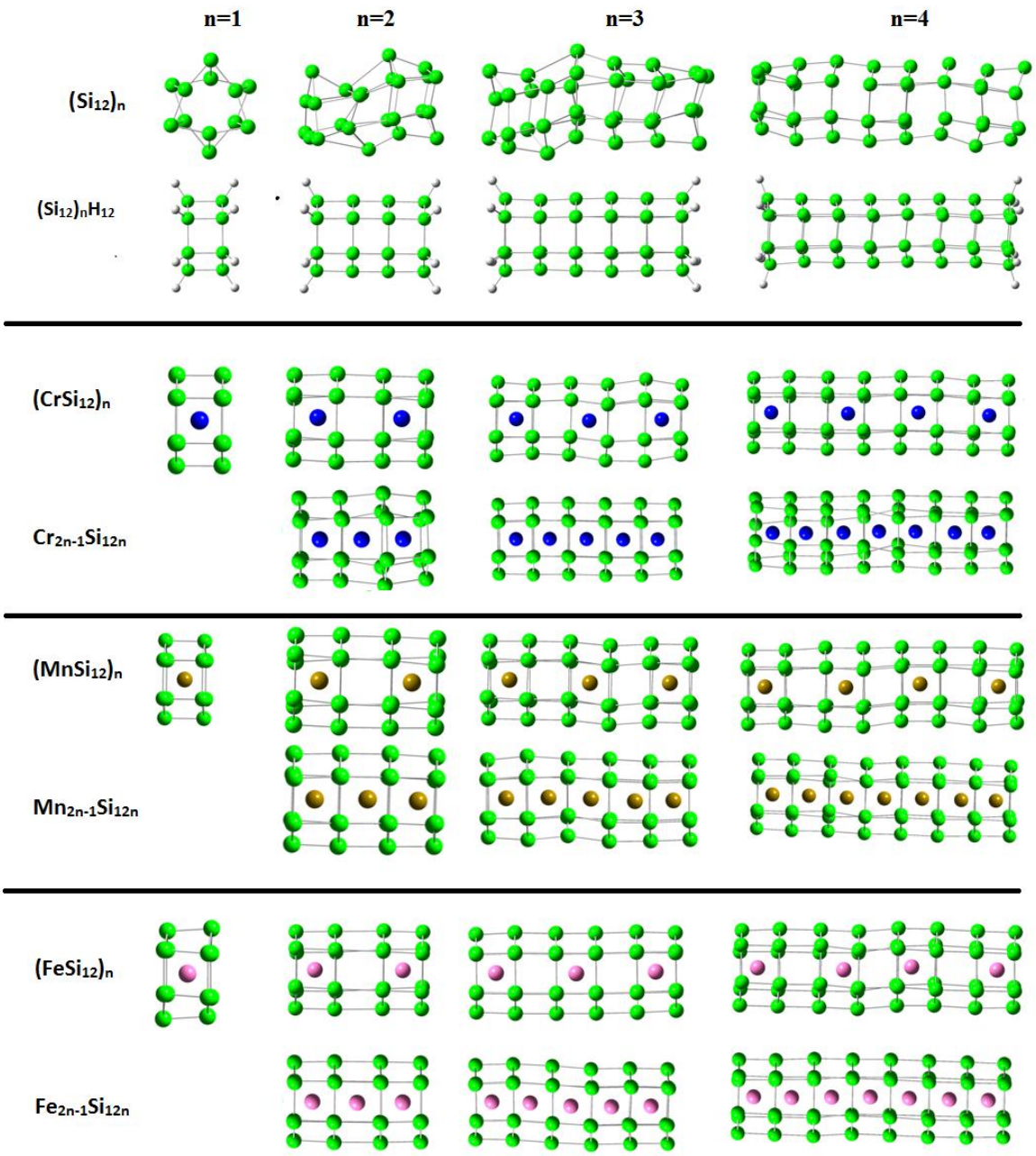
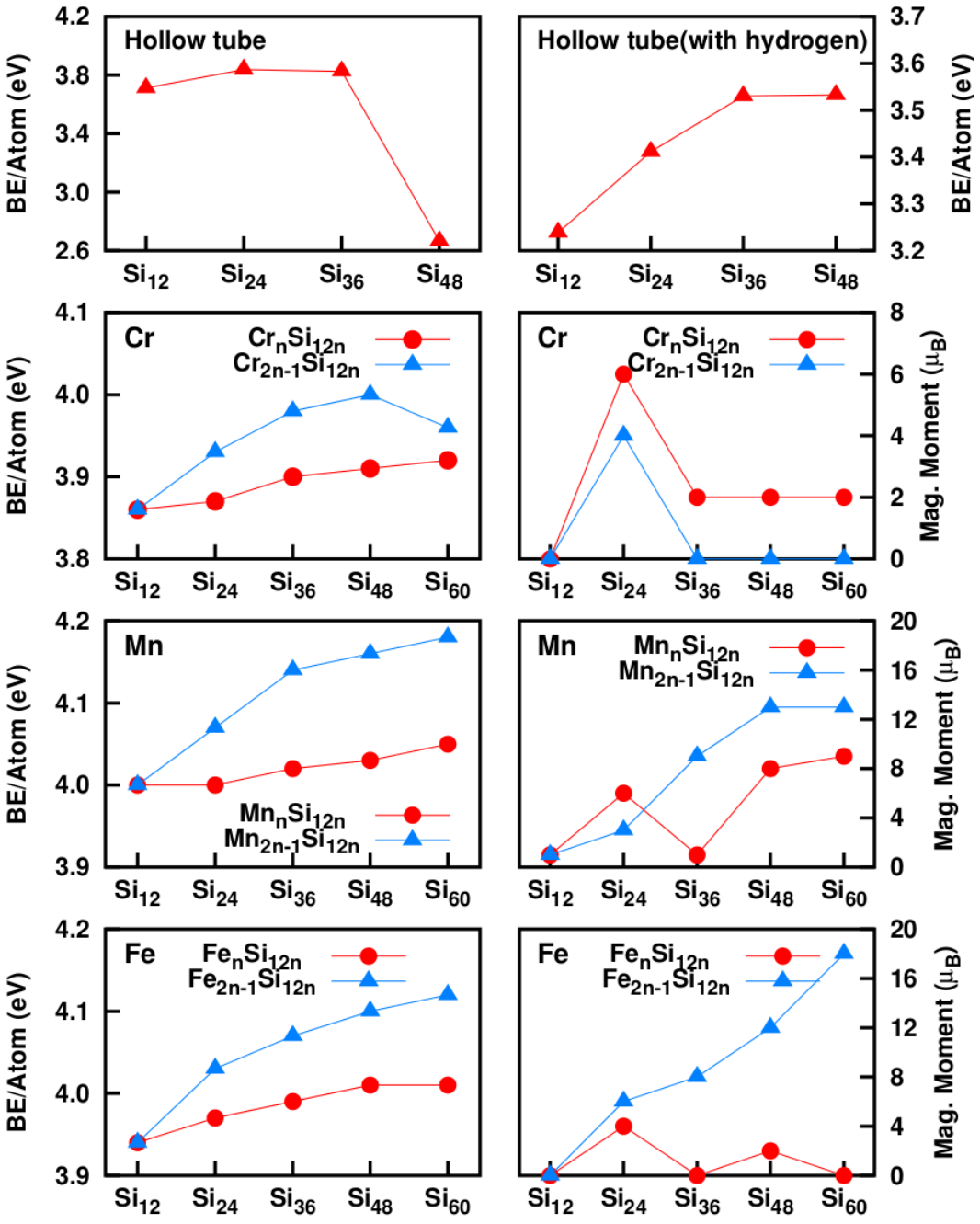
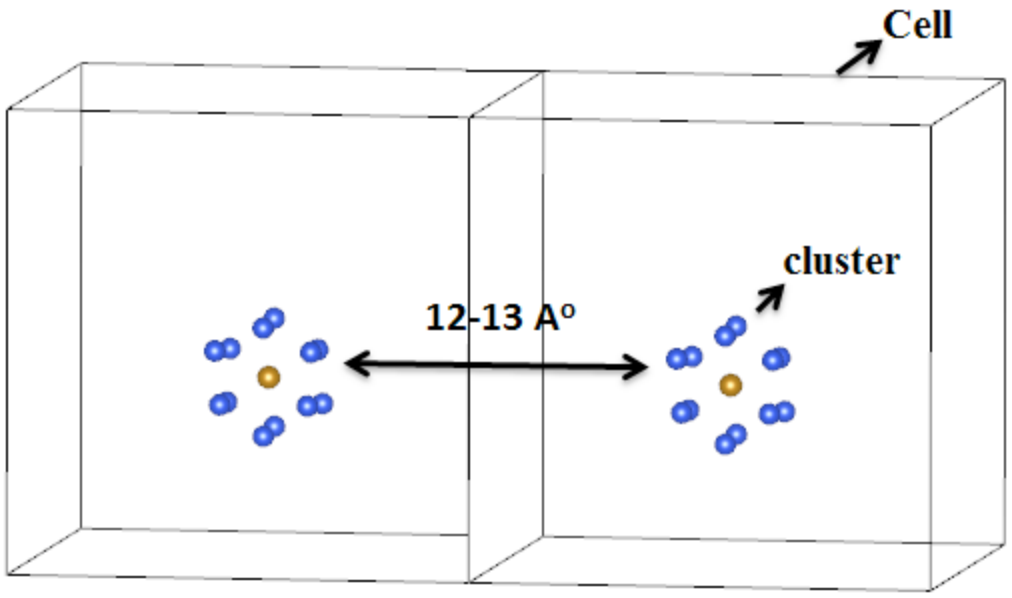
Total	0.205	0.572	7.408	8.386	Total	0.162	0.551	7.256	7.969	Total	0.029	-0.065	4.040	4.005



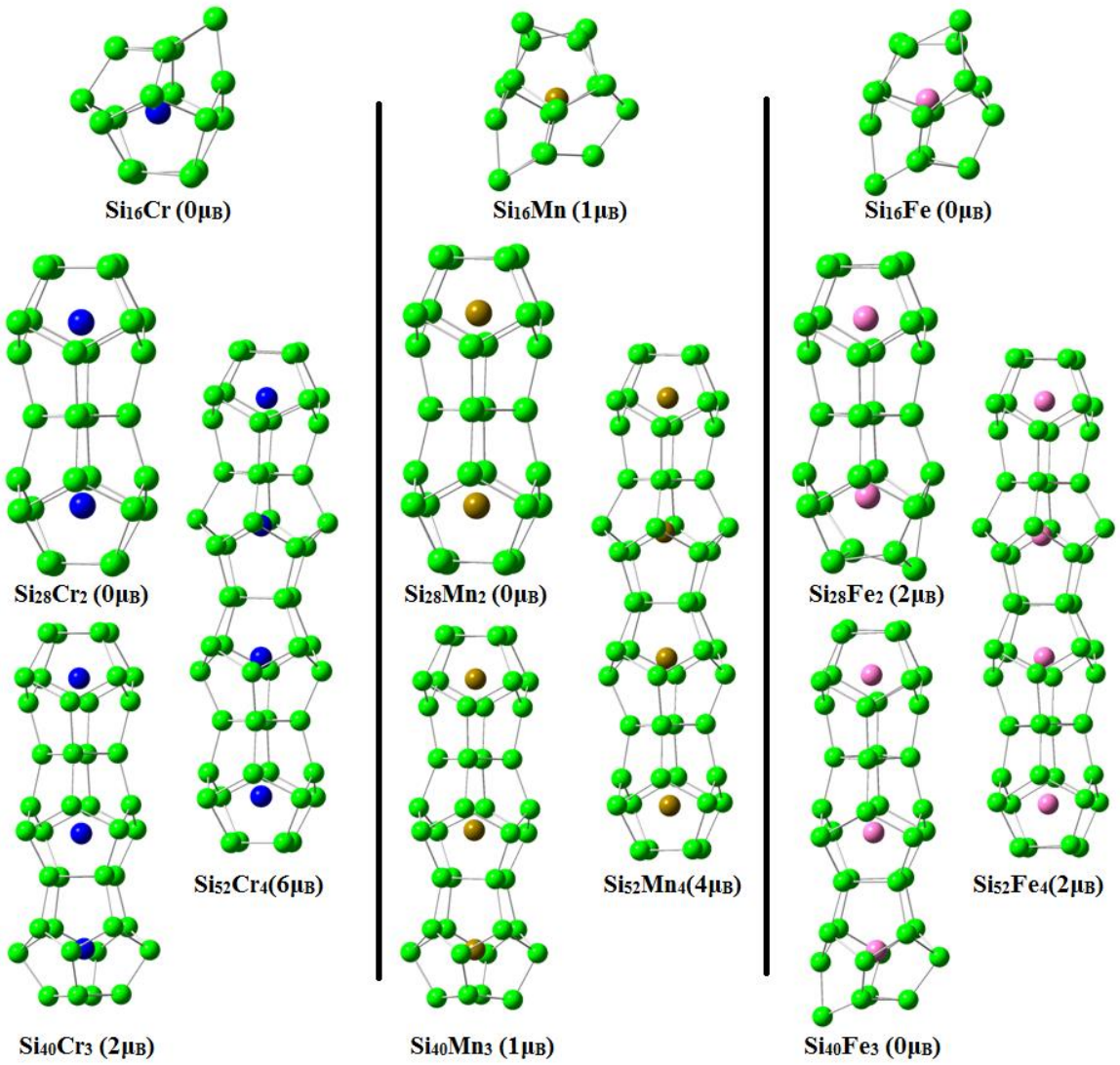
SI Fig. 1. Structures of hollow finite silicon nanotubes based on the most stable structures of empty Si_{12} and Si_{16} clusters as well as the effect of hydrogen termination and different transitional metal atom doping.



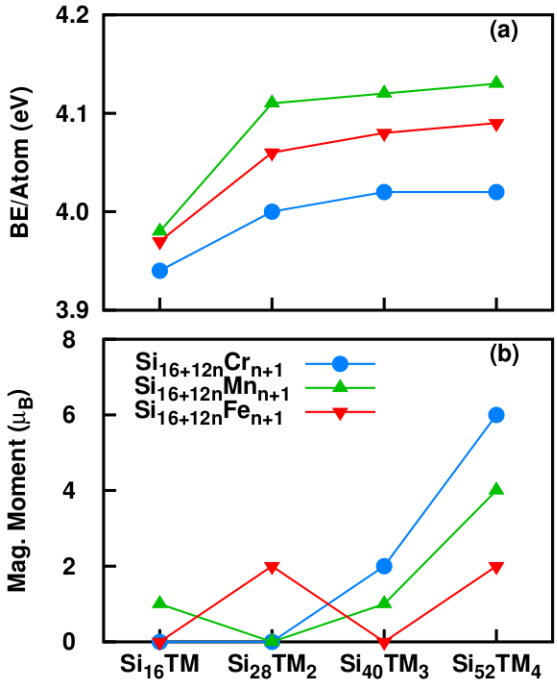
SI Fig. 2. Variation of average binding energy and corresponding magnetic moment of different TM_nSi_{12n} and $TM_{2n-1}Si_{12n}$ cluster assemblies shown in SI Fig. 1, where, TM = Cr, Mn and Fe.



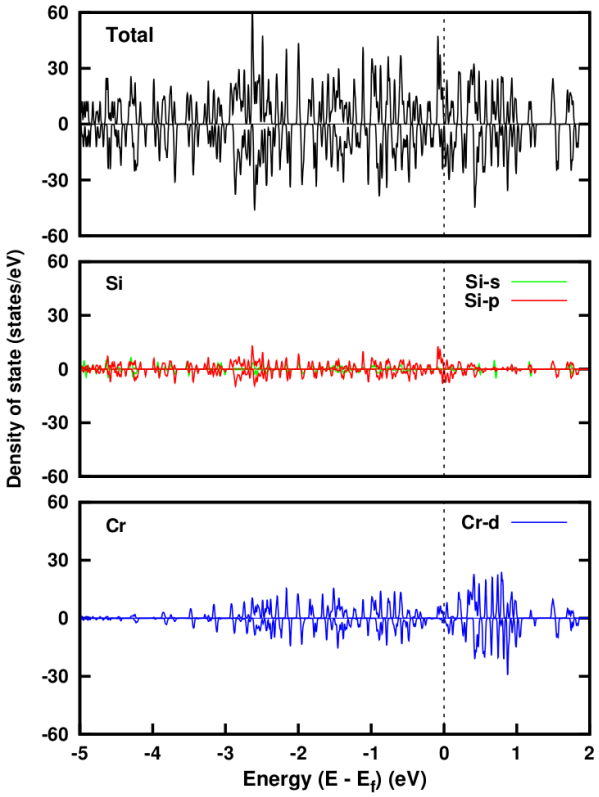
SI Fig. 3. Meaning of cluster and cell taken in the calculations based on the non-interacting system. Here each cluster is inside a cubic cell. We will get the actual picture if we extend the figure in all three (x-y-z) directions.



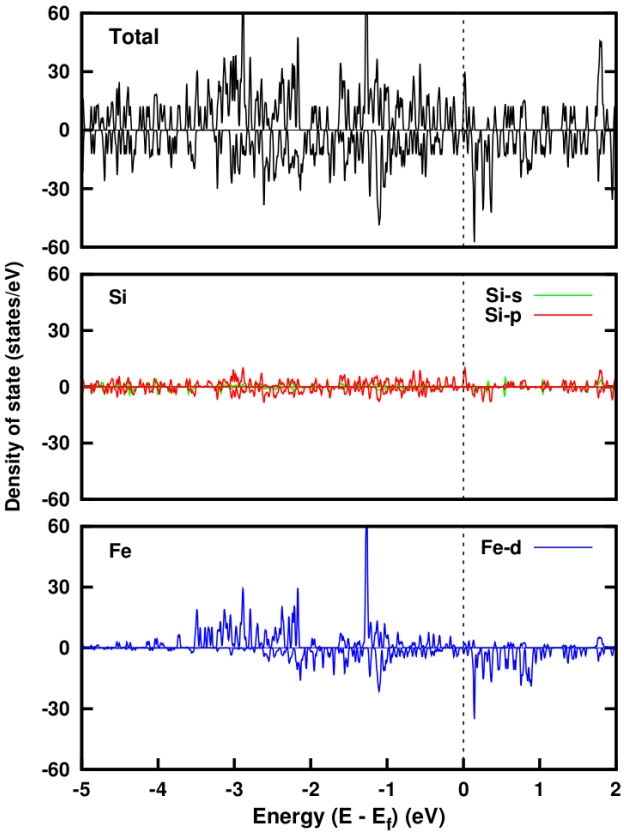
SI Fig. 4. Different TM-doped finite silicon nanotubes with $TMSi_{16}$, TM_2Si_{28}, TM_3Si_{40}, TM_4Si_{52} (where, TM=Cr, Mn and Fe). Green, brown, blue and pink spheres are representing Si, Mn, Cr and Fe respectively.



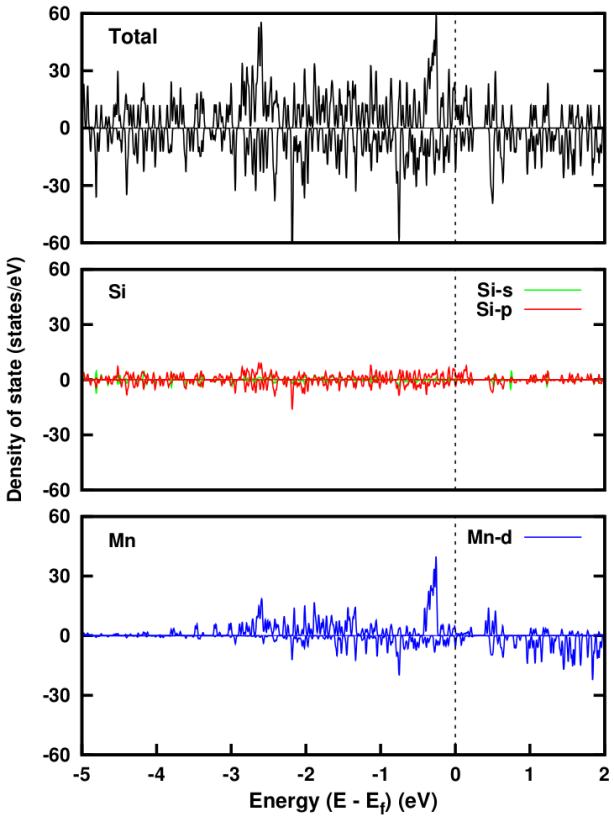
SI Fig. 5. Plots of (a) BE/atom and (b) magnetic moment versus different compositions of finite transition metal (TM= Cr,Mn and Fe) doped Type 2 silicon nanotubes.



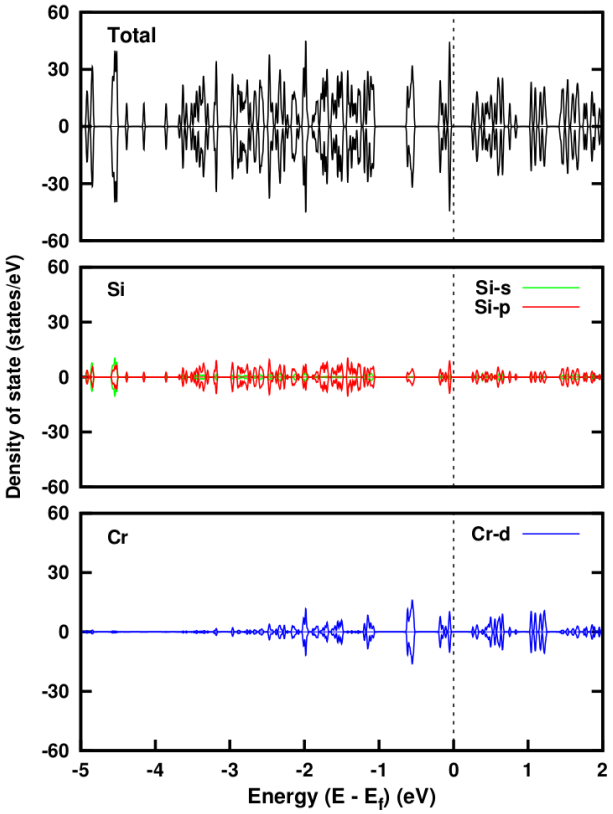
SI Fig. 6a. Variation of DOS and PDOS with energy near Fermi level for type 1 $(Cr_4Si_{24})_n$ infinite nanotubes.



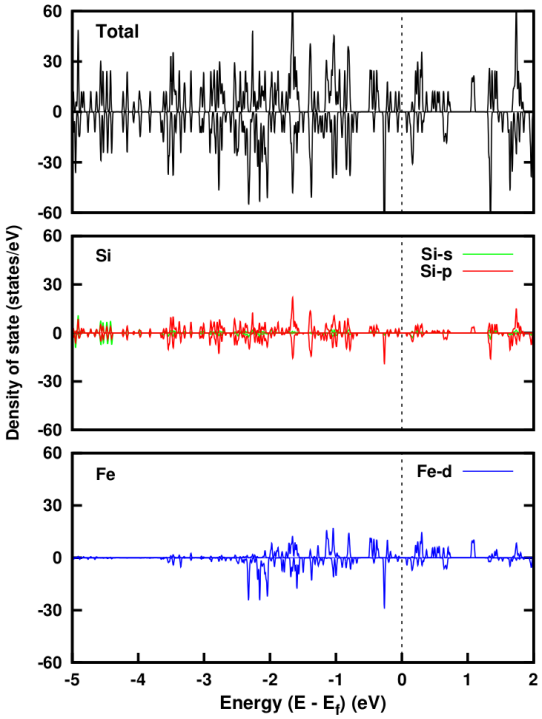
SI Fig. 6b. Variation of DOS and PDOS with energy near Fermi level for type 1 $(Fe_4Si_{24})_n$ infinite nanotubes.



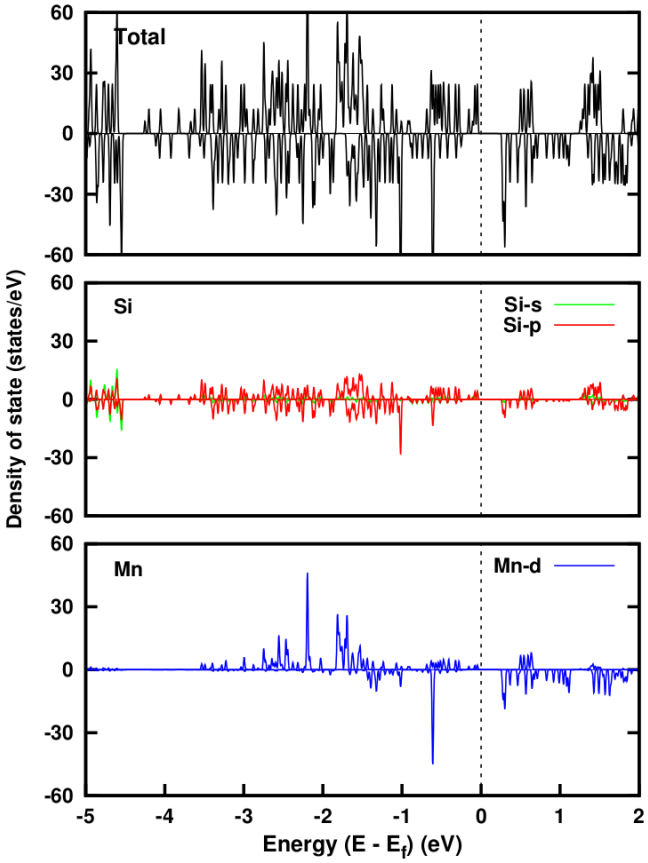
SI Fig. 6c. Variation of DOS and PDOS with energy near Fermi level for type 1 $(Mn_4Si_{24})_n$ infinite nanotubes.



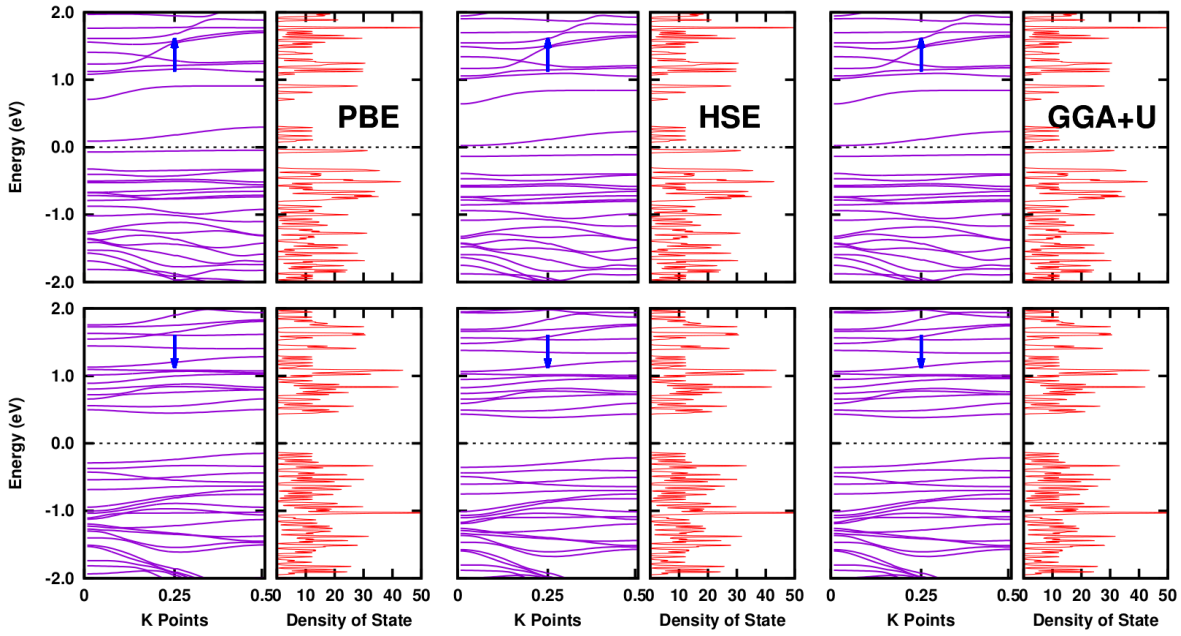
SI Fig. 7a. Variation of DOS and PDOS with energy near Fermi level for type 2 $(Cr_2Si_{24})_n$ infinite nanotubes.



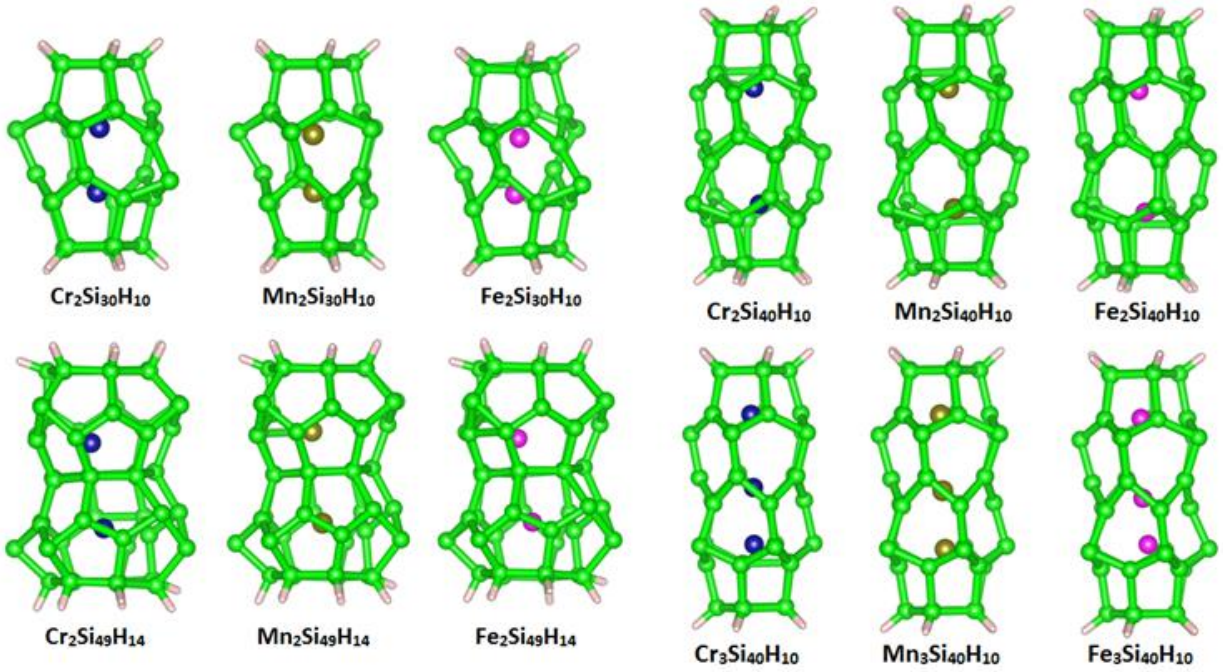
SI Fig. 7b. Variation of DOS and PDOS with energy near Fermi level for type 2 $(Fe_2Si_{24})_n$ infinite nanotubes.



SI Fig. 7c. Variation of DOS and PDOS with energy near Fermi level for type 2 $(Mn_2Si_{24})_n$ infinite nanotubes.

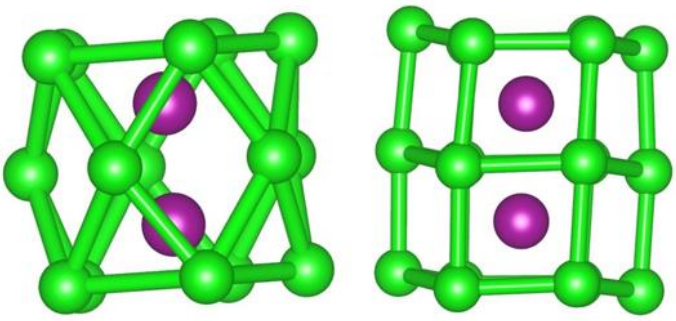


SI Fig. 8. Comparison of the band structure and DOS calculated using different approach as PBE, hybrid functional HSE and GGA+U in Mn doped Si Type 3 nanotube. It can be clearly seen that band gaps from each level of theory are almost same.



SI Fig. 9. Few more distorted structures.

Possibility of other nanotubes using the following units



$Si_{15}Mn_2$ $Si_{18}Mn_2$

Now the question arises here, “Does the ground state isomer in a particular size only the suitable candidate for making cluster assembled materials (finite nanotube) or a nanotube or something else also involved here?” For that we have calculated fukui function at each site as we have mentioned. Additionally, we have done the following exercise:

We agree with the reviewer that Si18Mn2 ball structure is the minimum energy structure, but as we have mentioned earlier that cluster requires un-saturated bonds on the surface to make bigger sized material (assembled material). To support this we have calculated BE/atom in four cases here

Average BE/atom of Si18Mn2 ball structure = 4.11 eV

Average BE/atom of Si18Mn2 tube structure= 4.04 eV

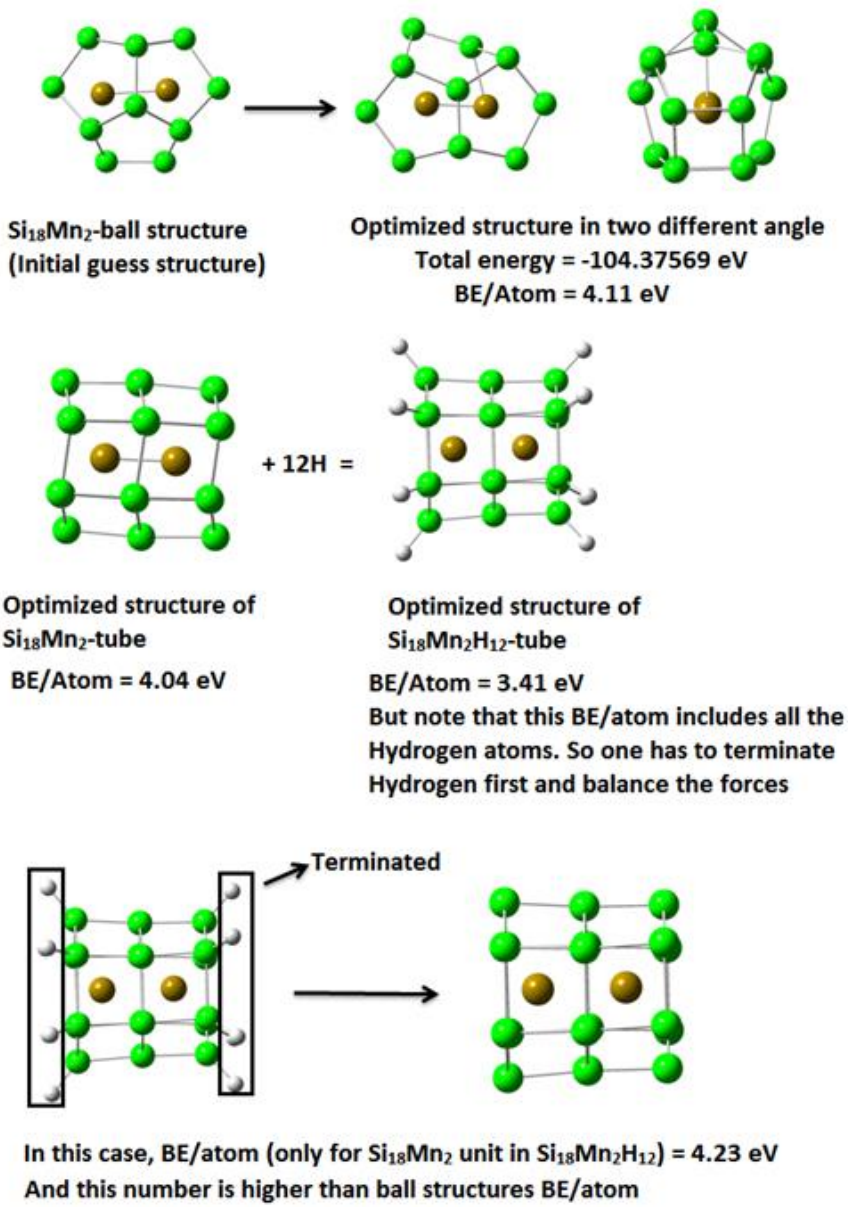
(Note that these two are the finite sized clusters, not in the infinite tube)

Average BE/atom of Si18Mn2H12 tube structure = 3.41 eV (Again note that it's the BE/atom included Hydrogen atoms in the clusters)

Average BE/atom of Si18Mn2 in Si18Mn2H12 tube structure by terminating Hydrogen atom in the cluster (after saturate all the forces on both the two ends of the tube) = 4.23 eV

So this is the proof that the composition Si18Mn2 holds tightly in the tube form rather than in a ball cluster structure.

The figure explanation is added below.



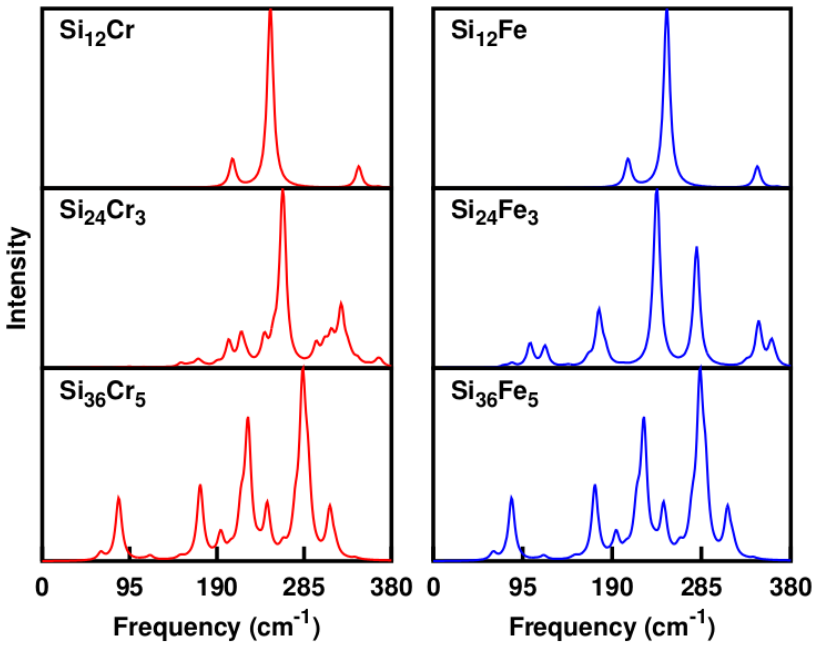
SI Fig.10. Pictorial representation of hydrogen termination effect on binding energies of the clusters

Confirmation of stability: Study of IR spectrum and Free energy variation of the clusters with the increase of the cluster size as functionalized assembled materials as finite nanotubes

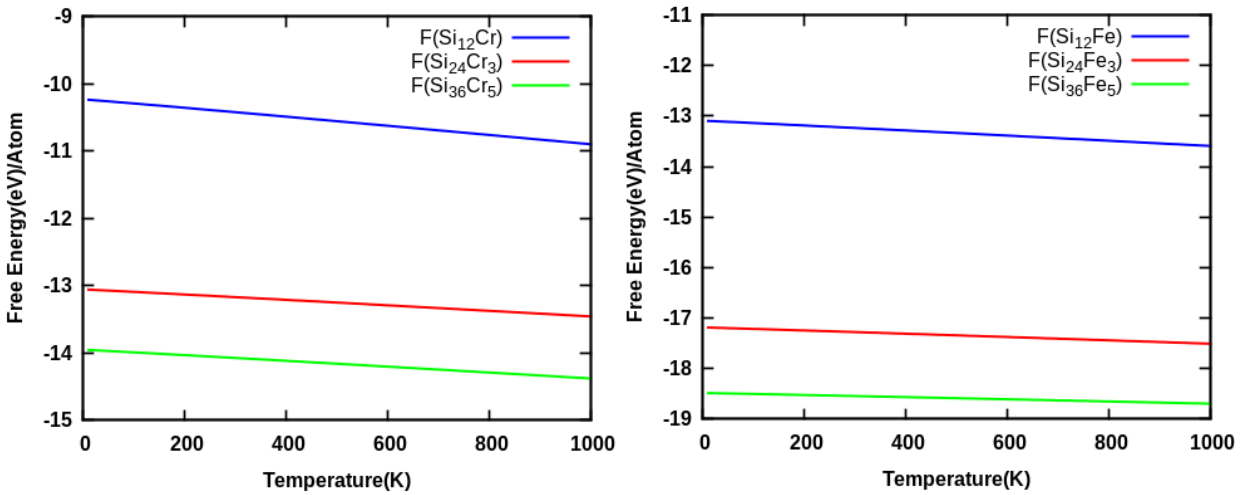
In order to provide spectroscopic fingerprints of the finite nanotubes, as an example we have calculated the IR spectrum of Type 1 nanoclusters ($Si_{12}Cr$, $Si_{24}Cr_3$, $Si_{36}Cr_5$ and $Si_{12}Fe$, $Si_{24}Fe_3$, $Si_{36}Fe_5$) as shown in Figure 11 . For the Cr doping, the spectrum shows three prominent peaks at 248 cm^{-1}, 260 cm^{-1} and 275 cm^{-1} for $Si_{12}Cr$, $Si_{24}Cr_3$, $Si_{36}Cr_5$ unites. Similarly for Fe doping, these pecks are 270 cm^{-1}, 238 cm^{-1} and 275 cm^{-1}. Using these vibration frequencies, we have also calculated the free energies including the vibrational entropies within the quasi-harmonic approximation (L. L. Boyer, Phys. Rev. Lett., 1979, 42, 584–587):

$$F(T) = E_0 + \frac{1}{2}\sum_i h\nu_i + k_B T \sum_i ln\left[1 - e^{-\frac{h\nu_i}{k_B T}}\right]$$

where E_0 is the total energy, and ν_i are the vibrational frequencies of the clusters. In the figure below, we demonstrate the variation of free energy with temperature from 0 to 1000K. It can be clearly seen in Fig 2 that the adding functionalized units on the end of the tubes makes minimized the energy. This indicates the stability of the bigger sized units.



SI Fig 11. IR frequency variation of type 1 functionalized clusters assemblies.



SI Fig. 12. Variation in free energies including the vibrational entropies within the quasi-harmonic approximation with temperature.