Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Structural and Electronic Properties of $NbSi_n^{-/0}$ (n = 3-12) Clusters: Anion Photoelectron Spectroscopy and *ab initio* Calculations

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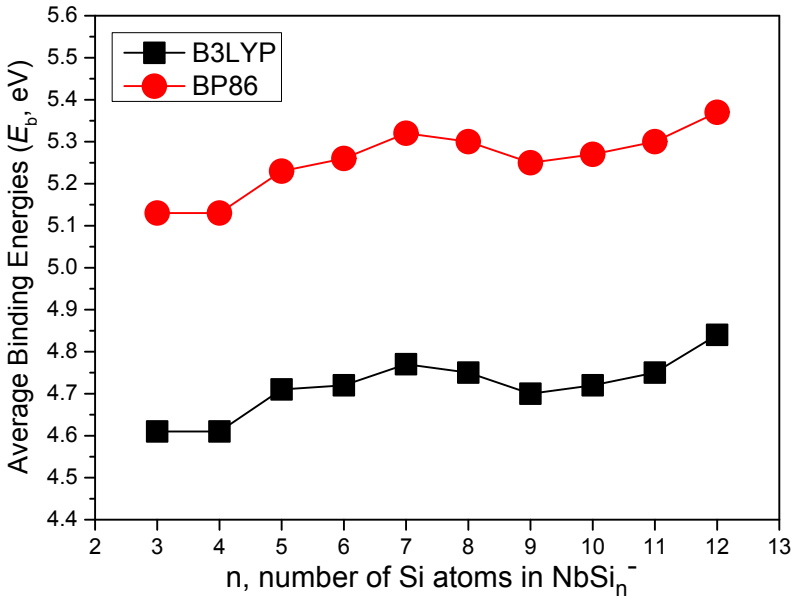

Fig. S1. The Average Binding Energies (E_b) per atom of $NbSi_n^-$ (n = 3−12) clusters as the function of the cluster sizes using the B3LYP and BP86 functionals. (E_b(n) = [E(Nb^-) + nE(Si) − E($NbSi_n^-$)]/(n + 1), the E represents the total energy including zero-point vibrational corrections.)

Average Binding Energies. In Fig. S1, we can see that $NbSi_{12}^-$ has the highest average binding energy (E_b) per atom, suggesting that $NbSi_{12}^-$ is very stable. Also, it is seen that the average binding energies (E_b) per atom are more overestimate by the BP86 functional than the B3LYP functional with average derivations of ~0.50 eV**.**

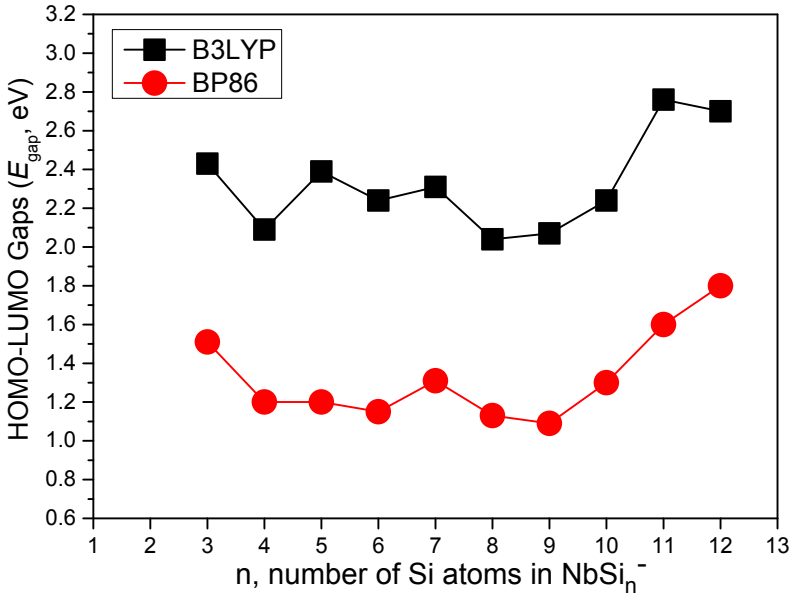

Fig. S2. The HOMO-LUMO Gaps (E_{gap}) of $NbSi_n^-$ (n = 3−12) clusters as the function of the cluster sizes using the B3LYP and BP86 functionals.

HOMO-LUMO Gaps. The HOMO-LUMO gaps obtained by the different functionals are similar to the E_b values with the increasing tendency along with the increasing Si atoms. The large HOMO-LUMO gaps suggest that these Nb atom doped silicon clusters are kinetically stable. Comparing the E_{gap} values obtained by the B3LYP functional with those calculated using the BP86 functional, we can found that the E_{gap} values calculated by the B3LYP functional are systematically larger than the BP86 functional with the average deviation of ~1.00 eV, which is consistent with the previous works (J. Am. Chem. Soc., 2010, **132**, 15589-15602; J. Comput. Chem., 2016, **37**, 2316-2323.).

Taking the E_b and E_{gap} values of $NbSi_n^-$ (n = 3-12) clusters into account, we can find that the $NbSi_{12}^-$ cluster has higher chemical stability and can be regarded as the magic cluster for the $NbSi_n^-$ clusters.

Table S1. Cartesian coordinates for stable isomers of $NbSi_{3-12}^{-/0}$ clusters.

$NbSi_3^-$

	3A				3B		
	X	Y	Z		X	Y	Z
Si	1.29922780	-0.75010952	0.90674907	Si	0.00000000	-1.93163364	0.52723281
Si	-0.00000000	1.50021904	0.90674907	Si	0.00000000	-0.00000000	1.71380992
Si	-1.29922780	-0.75010952	0.90674907	Si	-0.00000000	1.93163364	0.52723281
Nb	0.00000000	0.00000000	-0.92883186	Nb	0.00000000	-0.00000000	-0.94528708
Si	1.29922780	-0.75010952	0.90674907	Si	0.00000000	-1.93163364	0.52723281

$NbSi_4^-$

	4A				4B		
	X	Y	Z		X	Y	Z
Si	0.00487500	0.47485900	1.66374200	Si	0.04757008	1.54956768	-1.16540485
Si	-1.90584600	0.42551700	-0.26506000	Si	0.04757008	1.54956768	1.16540485
Si	1.90695900	0.41515600	-0.26885600	Si	-0.26581761	-0.38069594	-2.38892895
Si	0.00368800	1.80538800	-0.61638100	Si	-0.26581761	-0.38069594	2.38892895
Nb	-0.00330400	-1.06568000	-0.17532300	Nb	0.14923129	-0.79764075	0.00000000

$NbSi_5^-$

	5A				5B		
	X	Y	Z		X	Y	Z
Si	-0.00000000	-0.00000000	2.01855801	Si	0.76188400	1.13601600	-1.28732300
Si	0.00000000	1.88358649	0.39287762	Si	-1.64127800	1.10517800	-0.66272200
Si	0.00000000	-1.88358649	0.39287762	Si	-0.09979400	1.42150500	1.16297500
Si	1.88358649	0.00000000	0.39287762	Si	1.96660300	0.29747700	0.83945600
Si	-1.88358649	-0.00000000	0.39287762	Si	-1.84143900	-0.77826800	0.76250300
Nb	0.00000000	0.00000000	-1.21938499	Nb	0.29161800	-1.08650500	-0.27825500
	5C				5D		
	X	Y	Z		X	Y	Z
Si	1.79510646	1.62668973	0.00000000	Si	-1.16821200	-0.59393000	1.36733400
Si	-0.97537797	-0.78299878	-1.27950404	Si	-1.16821200	1.41360900	0.00000000
Si	-2.65496773	0.57418153	0.00000000	Si	-1.16821200	-0.59393000	-1.36733400
Si	-0.48403858	1.36905114	0.00000000	Si	-0.34703700	-2.34487300	0.00000000
Nb	1.12494705	-0.68523815	0.00000000	Si	0.98667000	2.30609100	0.00000000
Si	-0.97537797	-0.78299878	1.27950404	Nb	0.97829400	-0.06384200	0.00000000

$NbSi_6^-$

	6A				6B		
	X	Y	Z		X	Y	Z
Si	2.21292400	-0.00000100	-0.24924000	Si	0.01413033	2.29178469	-0.01717416
Si	0.85764300	-1.91584500	-0.11155900	Si	-1.79470381	1.05085692	-0.89209169
Si	0.64455400	0.00000000	1.74934400	Si	-1.99180892	-1.13365512	-0.01717416
Si	-1.34485200	-1.40570300	0.85896900	Si	-0.01271688	-2.07968755	-0.89209169
Si	0.85764600	1.91584400	-0.11155900	Si	1.97767860	-1.15812956	-0.01717416
Si	-1.34485000	1.40570600	0.85896800	Si	1.80742069	1.02883063	-0.89209169
Nb	-0.64299800	0.00000000	-1.02265600	Nb	-0.00000000	0.00000000	0.93142594

	6C				6D		
	X	Y	Z		X	Y	Z
Si	-0.62442932	2.40950015	0.17241431	Si	2.15732275	0.88359513	0.00000000
Si	-1.00537865	0.71100860	-1.38928204	Si	0.13365342	1.37128023	1.31932656
Si	1.48789119	1.49153000	-0.34819425	Si	1.10807290	-1.07768053	-1.31988075
Si	0.62442932	-2.40950015	0.17241431	Si	0.13365342	1.37128023	-1.31932656
Si	1.00537865	-0.71100860	-1.38928204	Si	1.10807290	-1.07768053	1.31988075
Si	-1.48789119	-1.49153000	-0.34819425	Nb	-0.93459270	-0.94693742	0.00000000
Nb	-0.00000000	0.00000000	1.06893786	Si	-1.90274192	1.30233334	0.00000000

$NbSi_7^-$

	7A				7B		
	X	Y	Z		X	Y	Z
Si	2.47578900	-0.00001600	-0.03749100	Si	-1.74359529	-1.18239877	0.00000000
Si	0.96934000	-1.95692700	-0.12031400	Si	0.48970539	-2.54317830	0.00000000
Si	0.84842600	0.00001900	1.68918100	Si	-0.05995874	-0.86479420	1.76811746
Si	-1.08484100	-1.47248200	1.04666900	Si	1.89791393	-0.27607064	0.00000000
Si	0.96934300	1.95693400	-0.12032700	Si	0.96720474	1.22233858	-1.71800286
Si	-1.08485900	1.47247900	1.04666900	Si	0.96720474	1.22233858	1.71800286
Si	-2.51112500	-0.00001400	-0.20212000	Si	-0.05995874	-0.86479420	-1.76811746
Nb	-0.19875700	0.00000200	-1.12760300	Nb	-0.83909074	1.12203201	0.00000000

	7C				7D		
	X	Y	Z		X	Y	Z
Si	0.49540907	-1.30512794	-1.96544355	Si	-0.80917600	-1.93806000	0.48085000
Si	1.83899917	-1.08806267	0.00000000	Si	-1.69993300	0.01215700	1.69569300
Si	0.49540907	-1.30512794	1.96544355	Si	0.63863300	0.01158000	1.49588700
Si	0.43736936	0.96510608	1.44275648	Si	-0.80923000	1.94440500	0.45397900
Si	-1.46262731	1.54077571	0.00000000	Si	1.26260400	-1.27811800	-0.73509900
Si	0.72980944	2.83095012	0.00000000	Si	1.26241200	1.26665400	-0.75448200
Si	0.43736936	0.96510608	-1.44275648	Nb	-0.92268700	-0.00780700	-1.09293800
Nb	-1.01592786	-0.88887620	0.00000000	Si	2.85684600	0.00424600	0.56391900

$NbSi_8^-$

	8A				8B		
	X	Y	Z		X	Y	Z
Si	-0.00000100	-1.97570700	0.73655600	Si	0.95545328	1.91006312	0.00000000
Si	0.00000100	1.97570800	0.73655400	Si	-3.06085883	0.94027947	0.00000000
Si	-2.14875300	-1.23966000	-0.42479000	Si	2.64097909	0.24626976	0.00000000
Si	-2.14874500	1.23966700	-0.42478800	Si	-2.04284908	-1.32512087	0.00000000
Si	2.14875100	-1.23966300	-0.42478500	Si	1.15667892	0.21278376	2.03004306
Si	2.14874700	1.23966400	-0.42479100	Si	1.15667892	0.21278376	-2.03004306
Si	1.37091600	0.00000100	1.63488200	Si	-1.02631397	0.64049586	1.25947626
Si	-1.37091600	-0.00000300	1.63488100	Si	-1.02631397	0.64049586	-1.25947626
Nb	0.00000000	-0.00000200	-1.03931900	Nb	0.42565193	-1.19222113	0.00000000

	8C				8D		
	X	Y	Z		X	Y	Z
Si	0.85225760	-0.92103912	2.50188837	Si	1.59801800	-0.18640700	1.65390100
Si	-0.39854162	1.14351745	1.94567505	Si	0.86042500	1.99611200	0.24135200
Si	0.40345038	2.28191121	0.00000000	Si	-1.06850600	1.26888100	-1.06494300
Si	0.85225760	-0.92103912	-2.50188837	Si	-0.07920000	-1.89047900	1.15345500
Si	-0.39854162	1.14351745	-1.94567505	Si	-1.91728000	-1.09008900	-0.65713800
Si	-1.11385732	-1.43061457	-1.24159686	Si	-2.98173600	0.79680600	0.47217500
Si	-1.11385732	-1.43061457	1.24159686	Si	-0.78345300	0.49488500	1.33920900
Si	-1.86585477	0.62274868	0.00000000	Si	2.66291300	0.61119600	-0.41788500
Nb	0.95012611	-0.16677619	0.00000000	Nb	0.58349900	-0.68323600	-0.92882300

$NbSi_9^-$

9A

	X	Y	Z
Si	2.11707454	-1.22229356	0.10479720
Si	2.18248137	1.26005621	-0.79445856
Si	-0.00000000	2.44458711	0.10479720
Si	-2.18248137	1.26005621	-0.79445856
Si	0.00000000	-2.52011242	-0.79445856
Si	-2.11707454	-1.22229356	0.10479720
Si	0.00000000	-1.46805816	1.57419389
Si	1.27137566	0.73402908	1.57419389
Si	-1.27137566	0.73402908	1.57419389
Nb	-0.00000000	-0.00000000	-0.90583395

9B

	X	Y	Z
Nb	-0.11770100	-0.28538900	-0.81163700
Si	-2.12411800	1.41608600	-0.21126800
Si	-2.66247500	-0.71925300	-1.15217000
Si	-1.81572000	-1.01964700	1.14493400
Si	0.48710300	-1.73252200	1.30714800
Si	-0.61088600	1.19830600	1.69038900
Si	0.54426100	2.08850100	-0.34571300
Si	1.68995600	0.34640400	1.34291200
Si	2.75948900	0.78900500	-0.72713200
Si	2.07708500	-1.53110000	-0.67216500

9C

	X	Y	Z
Nb	-0.41109000	-0.53661100	-0.00294000
Si	-2.86685700	0.48274500	-0.00488700
Si	-2.86647400	-1.69251200	0.00016000
Si	1.15134300	-0.81544200	1.96328100
Si	-1.15092800	1.99842700	0.00516700
Si	0.53177100	1.47147500	1.63586400
Si	0.53522100	1.48302100	-1.62423200
Si	2.26502200	0.90499200	0.00602200
Si	1.15574200	-0.80185900	-1.96830600
Si	2.44906500	-1.45934500	-0.00445900

9D

	X	Y	Z
Si	0.00000000	0.00000000	3.02132199
Si	-0.40759218	2.56233606	-0.23512185
Si	1.10923194	-0.71175179	-1.91445805
Si	1.09276486	1.67932821	-1.96600589
Si	-1.09276486	-1.67932821	-1.96600589
Si	0.40759218	-2.56233606	-0.23512185
Si	0.00430894	-2.08718308	2.03903685
Si	-1.10923194	0.71175179	-1.91445805
Si	-0.00430894	2.08718308	2.03903685
Nb	0.00000000	-0.00000000	0.38281399

$NbSi_{10}^-$

	10A				10B		
	X	Y	Z		X	Y	Z
Si	-0.63954400	2.64910800	-0.44197000	Si	2.15746200	-0.23199800	1.47154600
Si	-2.52477600	-1.12536400	-0.17107000	Si	2.02063800	-2.13762700	-0.00743500
Si	1.54548700	-2.09162400	-0.15570100	Si	-2.47610400	-1.65767400	-0.00595200
Si	-0.76149400	-2.62099400	-0.42809300	Si	2.15695800	-0.22268900	-1.47352700
Si	-0.35315300	1.27763200	1.70340900	Si	1.60052900	1.62587100	0.00547100
Si	1.79230300	-0.04236700	1.38599100	Si	-0.00879900	0.97914000	2.07084700
Si	2.54929700	-0.06071600	-0.94149200	Si	-2.19996800	0.02706500	1.63533700
Si	1.64019500	2.01613300	-0.15634100	Si	-2.20057900	0.03976200	-1.63427300
Si	-0.41930500	-1.24353300	1.70834900	Si	-0.00926800	0.99434700	-2.06399700
Si	-2.46831700	1.23820500	-0.16294100	Nb	-0.13899100	-0.60152500	-0.00224300
Nb	-0.12316400	0.00120200	-0.79907300	Si	-0.63382300	2.34541000	0.00855100

	10C				10D		
	X	Y	Z		X	Y	Z
Nb	0.27738300	0.01284900	-0.48409500	Si	0.62044580	-2.17031489	-1.23319436
Si	2.61275700	-1.35285900	0.13611000	Si	0.62044580	-2.17031489	1.23319436
Si	2.60620900	0.48842700	-1.36668200	Si	0.99041308	-0.37951764	2.73850395
Si	2.07539100	1.86300300	0.41942100	Si	-0.00158278	1.84359033	-2.06382763
Si	-0.12734700	1.77157900	1.37972100	Si	0.99041308	-0.37951764	-2.73850395
Si	0.47450600	-2.27939000	0.69131400	Si	-1.32424902	-0.34519054	-1.99985599
Si	-0.39983200	-0.52413900	2.14019900	Si	-1.59374311	-1.58309386	0.00000000
Si	-1.71850900	-2.01220800	-0.54405700	Si	-1.32424902	-0.34519054	1.99985599
Si	-2.40003400	-0.04797200	0.69319100	Si	-0.00158278	1.84359033	2.06382763
Si	-1.94519900	0.02697400	-1.80070700	Si	-0.09347662	2.94014097	0.00000000
Si	-1.99027800	2.02895600	-0.33080300	Nb	0.38174909	0.25532492	0.00000000

$NbSi_{11}^-$

	11A				11B		
	X	Y	Z		X	Y	Z
Si	1.30429990	-2.20683605	-0.28438689	Si	0.18662900	2.69231500	0.00658900
Si	0.00000000	-2.10452999	1.97950397	Si	-2.52863700	-0.16008700	-1.34767300
Si	0.00000000	0.00000000	3.06819593	Si	1.06338800	-2.41044100	-0.06160200
Si	-0.00000000	2.10452999	1.97950397	Si	-1.46900500	-2.16204100	-0.24453500
Si	-1.30429990	-2.20683605	-0.28438689	Si	0.76943800	1.11750300	1.82724400
Si	0.00000000	-1.20803006	-2.25619205	Si	2.40638900	-0.60157900	0.85506000
Si	2.07160305	-0.00000000	-1.30249485	Si	2.18555800	-0.64934900	-1.62174300
Si	1.30429990	2.20683605	-0.28438689	Si	2.29455900	1.48902900	-0.45680600
Si	-1.30429990	2.20683605	-0.28438689	Si	-2.47995700	-0.34107600	1.09762200
Si	-2.07160305	-0.00000000	-1.30249485	Si	-0.14029200	-1.07370000	1.88607000
Nb	0.00000000	0.00000000	0.39930793	Si	-2.10278200	1.85996900	-0.14229000
Si	-0.00000000	1.20803006	-2.25619205	Nb	-0.06326900	0.08176500	-0.61392900

	11C				11D		
	X	Y	Z		X	Y	Z
Nb	-0.00000000	0.00000000	0.63175101	Si	-1.98178900	2.35500221	0.00000000
Si	-2.66040613	-1.61257000	0.47281415	Si	-1.70106319	-2.28096880	0.00000000
Si	-2.39639630	0.22976727	-1.02710854	Si	-0.31235899	-2.02279102	-1.96824081
Si	-2.30794785	0.60181777	1.55461651	Si	0.86274603	0.15889091	-2.13803048
Si	-1.62027803	2.25952503	0.02204871	Si	-0.16839367	2.23369000	-1.62293924
Si	0.66385981	1.97753209	-0.87223373	Si	-0.16839367	2.23369000	1.62293924
Si	-0.66385981	-1.97753209	-0.87223373	Si	0.86274603	0.15889091	2.13803048
Si	0.00000000	0.00000000	-2.14951199	Si	-0.31235899	-2.02279102	1.96824081
Si	1.62027803	-2.25952503	0.02204871	Si	0.94823880	-2.55320591	0.00000000
Si	2.39639630	-0.22976727	-1.02710854	Si	2.22791489	-0.29686196	0.00000000
Si	2.30794785	-0.60181777	1.55461651	Si	1.58963698	1.96984207	0.00000000
Si	2.66040613	1.61257000	0.47281415	Nb	-0.62840910	0.02339216	0.00000000

$NbSi_{12}^-$

	12A				12B		
	X	Y	Z		X	Y	Z
Si	0.00000000	-2.41554021	-1.22437513	Si	2.37046300	0.00463800	1.32761700
Si	2.09191919	-1.20777011	-1.22437513	Si	-0.21741400	2.75519200	-0.74673200
Si	2.09191919	1.20777011	-1.22437513	Si	-2.05665900	-1.26510900	-1.34482500
Si	-0.00000000	2.41554021	-1.22437513	Si	-2.06191300	1.25851700	-1.34425900
Si	-2.09191919	1.20777011	-1.22437513	Si	0.05305100	0.00028000	2.18679500
Si	-2.09191919	-1.20777011	-1.22437513	Si	-1.18610800	-1.86117300	1.29961000
Si	0.00000000	-2.41554021	1.22437513	Si	-0.20716000	-2.75613200	-0.74743600
Si	2.09191919	-1.20777011	1.22437513	Si	2.13376300	-1.97344600	-0.18360800
Si	2.09191919	1.20777011	1.22437513	Si	-1.19417500	1.85748500	1.30129700
Si	0.00000000	2.41554021	1.22437513	Si	-2.62666400	-0.00490500	0.74359500
Si	-2.09191919	1.20777011	1.22437513	Si	2.12757100	1.97949400	-0.18788600
Si	-2.09191919	-1.20777011	1.22437513	Si	2.67044900	0.00262400	-1.19989500
Nb	-0.00000000	-0.00000000	0.00000000	Nb	0.06651600	0.00086600	-0.37706900

	12C				12D		
	X	Y	Z		X	Y	Z
Si	2.65650800	0.75021100	-0.77242300	Nb	-0.00010300	-0.17311800	-0.15330800
Si	1.10590400	2.56828900	-0.91754100	Si	-2.08965100	1.08620500	-1.21820500
Si	1.05921900	1.69139800	1.38195800	Si	-2.01136000	1.21619200	1.19697300
Si	2.03074400	-0.46385000	1.44756700	Si	-2.02418900	-1.46097400	-1.15691900
Si	2.29568600	-1.56104800	-0.82849500	Si	-1.96853300	-1.16806500	1.41721200
Si	-1.40692700	2.41413200	-0.90197300	Si	0.00536100	-2.43846000	-1.74355800
Si	0.16895800	-1.95821100	1.36260200	Si	0.00618000	-1.08726100	2.61946300
Si	0.17134500	-2.78562800	-0.94130900	Si	-0.00559200	2.22038100	-1.69536600
Si	-1.33657100	1.50735900	1.39709800	Si	-0.00683900	2.42451700	0.79828300
Si	-2.72411200	0.44116500	-0.75666700	Si	2.08360300	1.09581000	-1.21808600
Si	-1.91562200	-0.77824100	1.43814000	Si	2.00391000	1.22694700	1.19705300
Si	-2.10587600	-1.81928200	-0.84930100	Si	2.02972500	-1.44996200	-1.16034700
Nb	0.00025400	-0.00214900	-0.36183300	Si	1.97768500	-1.15834200	1.41247200

$NbSi_3$

3A

	X	Y	Z
Si	0.77571700	-1.33885100	-0.79068200
Si	0.76827600	1.34876900	-0.78133100
Si	1.23446400	-0.00323700	1.23903000
Nb	-0.94874100	-0.00228100	-0.11370100
Si	0.77571700	-1.33885100	-0.79068200

$NbSi_4$

4A

	X	Y	Z
Si	0.00000000	-1.12046252	1.54358536
Si	-0.00000000	1.12046252	1.54358536
Si	0.00000000	-2.39479795	-0.29838134
Si	-0.00000000	2.39479795	-0.29838134
Nb	0.00000000	-0.00000000	-0.85036390

4B

	X	Y	Z
Si	-0.00001500	0.49864900	1.64809800
Si	-1.91894900	0.50939700	-0.16398100
Si	1.91895500	0.50939400	-0.16396400
Si	0.00000700	1.61599700	-0.76966100
Nb	0.00000000	-1.06995400	-0.18797300

$NbSi_5$

5A

	X	Y	Z
Si	0.00000000	0.00000000	-2.03438401
Si	0.00000000	1.86893026	-0.40834072
Si	0.00000000	-1.86893026	-0.40834072
Si	-1.86893026	-0.00000000	-0.40834072
Si	1.86893026	0.00000000	-0.40834072
Nb	-0.00000000	-0.00000000	1.25253699

5B

	X	Y	Z
Si	0.75923000	-1.61416000	0.00644000
Si	0.72301200	0.53754600	1.27764800
Si	-0.77756400	1.93297500	-0.00726500
Si	0.71677000	0.51959600	-1.27231700
Nb	-1.39952000	-0.47333800	0.00086000
Si	2.67714700	0.01024600	-0.00702600

5C

	X	Y	Z
Si	0.99879600	0.86267700	-1.34884900
Si	-1.23154600	1.36363500	-0.67058600
Si	0.25473500	1.41931100	1.16843200
Si	2.03850000	-0.04852800	0.78220800
Si	-2.11967300	-0.29338900	0.64124700
Nb	0.02021100	-1.12809500	-0.19547100

5D

	X	Y	Z
Si	1.72359836	1.69879346	0.00000000
Si	-0.94098916	-0.78028905	-1.23800566
Si	-2.69932789	0.49244238	0.00000000
Si	-0.52323370	1.39480293	0.00000000
Nb	1.15452487	-0.69148042	0.00000000
Si	-0.94098916	-0.78028905	1.23800566

$NbSi_6$

6A

	X	Y	Z
Si	2.21993800	0.00000000	-0.44565700
Si	0.84366100	-1.91027100	-0.18344500
Si	0.83085000	0.00000000	1.65047200
Si	-1.18608800	-1.43510600	0.99069800
Si	0.84366100	1.91027100	-0.18344500
Si	-1.18608800	1.43510600	0.99069800
Nb	-0.80788000	0.00000000	-0.96269600

6B

	X	Y	Z
Si	0.56645000	1.92667600	0.89387400
Si	-0.94863900	1.23542700	-0.79143700
Si	0.73566800	-1.83769500	0.98109600
Si	-0.75904500	-1.18835500	-0.92980100
Si	-0.93477800	-0.03737200	1.41686400
Si	-2.80189200	-0.15064600	-0.20427700
Nb	1.41442200	0.01774400	-0.46654800

6C

	X	Y	Z
Si	1.18452000	1.69015800	0.00000600
Si	-0.72651200	1.18090900	1.36766200
Si	1.61981100	-0.29235300	-1.36465100
Si	-0.72652100	1.18093900	-1.36764600
Si	1.61981700	-0.29236400	1.36464400
Nb	-0.20848800	-1.19376700	-0.00000700
Si	-2.36054400	0.02874400	0.00000400

6D

	X	Y	Z
Si	1.18452000	1.69015800	0.00000600
Si	-0.72651200	1.18090900	1.36766200
Si	1.61981100	-0.29235300	-1.36465100
Si	-0.72652100	1.18093900	-1.36764600
Si	1.61981700	-0.29236400	1.36464400
Nb	-0.20848800	-1.19376700	-0.00000700
Si	-2.36054400	0.02874400	0.00000400

$NbSi_7$

7A

	X	Y	Z
Si	-1.01835820	1.08683974	1.54249446
Si	0.12800622	-0.96608246	-1.98345171
Si	0.17074488	2.40577194	0.00000000
Si	-0.10596104	-2.35056795	0.00000000
Si	0.12800622	-0.96608246	1.98345171
Si	-1.76962039	-0.72673228	0.00000000
Si	-1.01835820	1.08683974	-1.54249446
Nb	1.19106497	0.14683253	0.00000000

7B

	X	Y	Z
Si	-2.35008200	0.00000300	0.10526300
Si	-0.96492100	1.98409900	-0.12664600
Si	-0.72709400	-0.00000200	1.77024100
Si	1.08642100	1.54177000	1.01889200
Si	-0.96492400	-1.98409800	-0.12664500
Si	1.08642000	-1.54177100	1.01889000
Si	2.40629300	0.00000000	-0.17212400
Nb	0.14610800	0.00000000	-1.19098000

7C

	X	Y	Z
Si	-0.60142907	-0.77380384	1.94262949
Si	-1.51540758	-1.85974317	0.00000000
Si	-1.47894397	0.58255584	0.00000000
Si	-0.60142907	-0.77380384	-1.94262949
Si	0.69608305	1.23226330	1.29289917
Si	0.69608305	1.23226330	-1.29289917
Nb	1.16476125	-0.84876774	0.00000000
Si	-0.59998232	2.84621398	0.00000000

7D

	X	Y	Z
Si	-1.30288300	2.04822000	-0.56524000
Si	-1.25818300	-0.00001300	-1.63040200
Si	-1.30288700	-2.04823200	-0.56520800
Si	0.93933300	-1.37938300	-0.51787800
Si	1.57540500	-0.00000600	1.40965900
Si	2.87245100	-0.00002900	-0.74458500
Si	0.93936500	1.37941400	-0.51786900
Nb	-0.84088800	0.00000900	1.06930000

$NbSi_8$

	8A				8B		
	X	Y	Z		X	Y	Z
Si	-0.00000100	-2.02931200	0.70849600	Si	1.53418800	-0.35572900	1.67653400
Si	0.00000100	2.02931200	0.70849500	Si	0.69435600	1.98564400	0.40837100
Si	-2.10263500	-1.29364000	-0.38056300	Si	-1.11314800	1.30835400	-1.00293200
Si	-2.10263400	1.29364100	-0.38056100	Si	-0.01061200	-2.04253500	0.89001200
Si	2.10263500	-1.29364100	-0.38056000	Si	-1.77982300	-1.06481400	-0.64998700
Si	2.10263500	1.29364000	-0.38056300	Si	-3.05607800	0.65450100	0.47839300
Si	1.26397700	0.00000100	1.61248100	Si	-0.85570600	0.31557800	1.38769700
Si	-1.26397800	0.00000000	1.61248000	Si	2.64072800	0.76362100	-0.17785800
Nb	0.00000000	0.00000000	-1.06526500	Nb	0.66452000	-0.53426100	-1.02788300

	8C				8D		
	X	Y	Z		X	Y	Z
Si	2.55847200	-0.70789700	-0.78652200	Si	-0.70599600	0.00003500	1.88357900
Si	1.90150000	1.21371600	0.54096500	Si	3.10025000	0.00001700	0.89727100
Si	0.00000000	2.17891900	-0.49353800	Si	-2.64617300	0.00001100	0.55313600
Si	-2.55847100	-0.70789800	-0.78652200	Si	1.99875000	-0.00002300	-1.25102700
Si	-1.90150100	1.21371500	0.54096400	Si	-1.21463200	2.00949900	0.15403700
Si	-1.20202300	-1.49603600	1.03850400	Si	-1.21463200	-2.00949200	0.15411200
Si	1.20202400	-1.49603700	1.03850200	Si	1.01719500	1.32004600	0.60269900
Si	0.00000000	0.54398800	1.85452000	Si	1.01719600	-1.32002300	0.60274700
Nb	0.00000000	-0.25352600	-1.00624900	Nb	-0.46164400	-0.00002300	-1.22809200

$NbSi_9$

	9A				9B		
	X	Y	Z		X	Y	Z
Si	-1.23742800	-2.22556600	0.01449900	Nb	-0.12693800	-0.29662000	-0.87468200
Si	2.07845200	-1.63396400	-0.67454800	Si	-2.02337200	1.46695300	-0.29998000
Si	2.46848300	0.57109200	0.30936600	Si	-2.72508400	-0.78470900	-0.98535700
Si	0.92288900	2.12934300	-0.82894800	Si	-1.78698200	-0.89985200	1.21054400
Si	-2.52335900	-0.01759500	-0.82785000	Si	0.44384600	-1.70638300	1.33386200
Si	-1.38806900	2.02396700	0.10900700	Si	-0.59648200	1.28079700	1.62523000
Si	-1.53249000	-0.23753800	1.53981100	Si	0.62034700	2.05757400	-0.42337000
Si	0.72052300	-1.28016200	1.46377000	Si	1.63855800	0.35388900	1.38335500
Si	0.48435200	1.22200900	1.64129400	Si	2.81318800	0.68413100	-0.64337600
Nb	0.00227000	-0.18834700	-0.93779500	Si	1.98772800	-1.58372600	-0.63933900

	9C				9D		
	X	Y	Z		X	Y	Z
Si	-2.27907800	1.12192100	-0.64194400	Si	-2.46885500	-0.40838800	-0.81078800
Si	-0.40029200	-2.20627500	0.11359700	Si	0.94238100	-2.09938300	0.43060100
Si	2.71239900	0.28819600	0.45273800	Si	2.45783100	1.58992900	0.08478100
Si	1.96104700	-1.59313900	-0.84186100	Si	2.54758400	-0.73655000	-0.65501400
Si	-1.30699200	-0.14435500	1.54116400	Si	-1.29508200	0.13770600	1.49858500
Si	1.40855200	2.20756300	-0.17360500	Si	0.13528400	2.07675900	0.16646000
Si	-0.74656900	2.10566400	0.88306600	Si	-2.26919700	1.86651400	0.08646000
Si	1.00154600	-1.00197100	1.59130700	Si	1.31045400	0.02226700	1.60346200
Si	-2.61129400	-1.24538900	-0.21849100	Si	-1.46910400	-2.08030900	0.56082300
Nb	0.08901300	0.15973100	-0.92399000	Nb	0.03711800	-0.12584400	-1.01256500

$NbSi_{10}$

	10A				10B		
	X	Y	Z		X	Y	Z
Si	-2.12778978	-0.18328592	-1.44242630	Nb	0.51420290	-0.25202500	0.00000000
Si	-2.10782553	-2.11602264	0.00000000	Si	-0.26531597	-2.35208368	-1.59922415
Si	2.52087335	-1.68356346	0.00000000	Si	1.40009480	-2.66802604	0.00000000
Si	-2.12778978	-0.18328592	1.44242630	Si	-0.26531597	-2.35208368	1.59922415
Si	-1.54708651	1.67203850	0.00000000	Si	-1.10290410	-0.18511431	2.04507065
Si	0.00162701	1.03511953	-2.06534425	Si	-1.10290410	-0.18511431	-2.04507065
Si	2.15054019	0.03506194	-1.60530055	Si	-2.17900408	0.47584510	0.00000000
Si	2.15054019	0.03506194	1.60530055	Si	0.43248701	1.73504736	-1.96268975
Si	0.00162701	1.03511953	2.06534425	Si	-0.69024600	2.50358904	0.00000000
Nb	0.12079209	-0.65814507	0.00000000	Si	1.83433698	2.03140595	0.00000000
Si	0.73138134	2.28283108	0.00000000	Si	0.43248701	1.73504736	1.96268975

	10C				10D		
	X	Y	Z		X	Y	Z
Si	-1.20863600	-2.28247100	-0.83756100	Si	-1.18013100	-2.30190700	-0.36780400
Si	2.86399500	-0.46554300	-0.20024900	Si	1.19016200	-2.30760200	-0.36541900
Si	-0.01072800	2.70366600	0.20148200	Si	2.68480300	-0.57320100	-0.93326300
Si	2.04347600	1.66294300	-0.47244500	Si	-2.04264700	1.84041800	-0.09121800
Si	-0.68892000	-1.56329700	1.41461900	Si	-2.69567200	-0.58147900	-0.92114700
Si	-1.12501500	0.87948400	1.63741700	Si	-1.96333300	-0.13592500	1.31360000
Si	-1.92598200	1.69635700	-0.73175600	Si	0.01930400	-1.29600500	1.69863800
Si	-2.61115800	-0.46531700	-0.04934300	Si	1.98432600	-0.10427000	1.29998100
Si	1.22929100	0.04373500	1.67294400	Si	2.01812700	1.87515600	-0.09398000
Si	1.27586200	-2.26245100	-0.08776500	Si	-0.02048600	2.92162700	0.16614300
Nb	0.05388800	0.01806100	-0.86982400	Nb	0.00189400	0.22645500	-0.58237600

$NbSi_{11}$

	11A				11B		
	X	Y	Z		X	Y	Z
Si	0.16753900	2.73389200	-0.06613800	Si	-2.35348112	-0.38897321	-1.55003980
Si	-2.49200500	-0.14043700	-1.32765500	Si	2.35348112	0.38897321	-1.55003980
Si	1.11569700	-2.42162300	-0.06222600	Si	1.83948989	2.16682303	-0.06467423
Si	-1.38704000	-2.19987700	-0.25881000	Si	-0.44314301	2.01862791	0.82831999
Si	0.55942500	1.15042000	1.78843400	Si	-2.51684612	1.72152679	-0.37001980
Si	2.32255500	-0.54991200	0.97192100	Si	-1.83948989	-2.16682303	-0.06467423
Si	2.26972700	-0.67620200	-1.47070900	Si	0.44314301	-2.01862791	0.82831999
Si	2.29848500	1.54954500	-0.31122600	Si	2.51684612	-1.72152679	-0.37001980
Si	-2.51095300	-0.44349500	1.05073000	Si	2.35178411	0.13878207	1.09316673
Si	-0.15800500	-1.10759400	1.85621300	Si	-0.00000000	0.00000000	2.14678796
Si	-2.07178800	1.84832400	-0.02755900	Si	-2.35178411	-0.13878207	1.09316673
Nb	-0.03880300	0.08774200	-0.73174800	Nb	0.00000000	0.00000000	-0.68908704

	11C				11D		
	X	Y	Z		X	Y	Z
Si	-2.35348112	-0.38897321	-1.55003980	Si	0.53160900	2.22313900	-1.32429900
Si	2.35348112	0.38897321	-1.55003980	Si	-1.57807900	2.17228800	-0.03772900
Si	1.83948989	2.16682303	-0.06467423	Si	-3.12243000	0.39037800	-0.26401200
Si	-0.44314301	2.01862791	0.82831999	Si	-2.44968200	-1.76368800	-0.22018400
Si	-2.51684612	1.72152679	-0.37001980	Si	0.06599000	1.77422900	1.82668500
Si	-1.83948989	-2.16682303	-0.06467423	Si	2.03138700	1.39587000	0.42982500
Si	0.44314301	-2.01862791	0.82831999	Si	1.63199200	0.11958600	-1.93610700
Si	2.51684612	-1.72152679	-0.37001980	Si	1.13362600	-2.16153500	-1.12438800
Si	2.35178411	0.13878207	1.09316673	Si	-0.37962000	-2.48350600	0.79461300
Si	-0.00000000	0.00000000	2.14678796	Si	0.76508000	-0.46823000	2.10148100
Si	-2.35178411	-0.13878207	1.09316673	Nb	-0.38498600	-0.10141300	-0.24039400
Nb	0.00000000	0.00000000	-0.68908704	Si	2.49758500	-0.90153600	0.45812600

$NbSi_{12}$

	12A				12B		
	X	Y	Z		X	Y	Z
Si	0.00000000	2.43034174	-1.20510123	Si	-1.29732385	2.37477794	0.00000000
Si	-2.10473768	1.21517087	-1.20510123	Si	0.61519779	-0.18796343	-2.67039788
Si	-2.10473768	-1.21517087	-1.20510123	Si	1.36428885	-2.10363219	1.26999322
Si	0.00000000	-2.43034174	-1.20510123	Si	1.36428885	-2.10363219	-1.26999322
Si	2.10473768	-1.21517087	-1.20510123	Si	-2.16920904	0.08435301	0.00000000
Si	2.10473768	1.21517087	-1.20510123	Si	-1.33243805	-1.23616092	1.80442031
Si	0.00000000	2.43034174	1.20510123	Si	0.61519779	-0.18796343	2.67039788
Si	-2.10473768	1.21517087	1.20510123	Si	0.16806725	2.21886797	1.98271696
Si	-2.10473768	-1.21517087	1.20510123	Si	-1.33243805	-1.23616092	-1.80442031
Si	-0.00000000	-2.43034174	1.20510123	Si	-0.68734626	-2.66340112	0.00000000
Si	2.10473768	-1.21517087	1.20510123	Si	0.16806725	2.21886797	-1.98271696
Si	2.10473768	1.21517087	1.20510123	Si	1.25445117	2.60705672	0.00000000
Nb	0.00000000	0.00000000	-0.00000000	Nb	0.43336096	0.07349179	0.00000000

	12C				12D		
	X	Y	Z		X	Y	Z
Nb	0.00000000	-0.00000000	-0.17164904	Si	0.82371482	0.64442868	2.65692323
Si	1.21654352	2.06246794	1.17140283	Si	0.70110806	2.56505082	1.28862140
Si	-1.21654352	2.06246794	1.17140283	Si	-1.45771601	1.46952799	1.20499113
Si	1.26686274	2.01430188	-1.26123310	Si	-1.36392523	-0.72784209	1.95846893
Si	-1.26686274	2.01430188	-1.26123310	Si	0.89393467	-1.67274430	2.40315402
Si	2.29997982	-0.00000000	-1.90792588	Si	0.70110806	2.56505082	-1.28862140
Si	-2.29997982	-0.00000000	-1.90792588	Si	-1.40839817	-2.02584690	0.00000000
Si	1.23405168	-0.00000000	2.33572558	Si	0.86931879	-2.57309007	0.00000000
Si	-1.23405168	-0.00000000	2.33572558	Si	-1.45771601	1.46952799	-1.20499113
Si	1.21654352	-2.06246794	1.17140283	Si	0.82371482	0.64442868	-2.65692323
Si	-1.21654352	-2.06246794	1.17140283	Si	-1.36392523	-0.72784209	-1.95846893
Si	1.26686274	-2.01430188	-1.26123310	Si	0.89393467	-1.67274430	-2.40315402
Si	-1.26686274	-2.01430188	-1.26123310	Nb	0.45967098	0.01108696	0.00000000