Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Endohedral group-14-element clusters $TM@E_9$ (TM = Co, Ni, Cu; E = Ge, Sn, Pb) and their low-dimensional nanostructures: A first-principles study

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To select the optimum functional, we test M062X, PBE0, B3LYP as well as X3LYP functionals for empty $[Ge_9]^{4-}$, $[Sn_9]^{4-}$, and $[Pb_9]^{4-}$ cluster. We divided E-E bonds of these $[E_9]^{4-}$ structures into four groups as shown in Fig.S1, and comparing the bond distances with experiments. We found the PBE0 shows better precision and efficiency for all three clusters, as shown in Table S1. We thus selected PBE0 functional for the geometric optimized calculations.

Table S1 The optimized results of $[Ge_9]^{4-}$, $[Sn_9]^{4-}$ and $[Pb_9]^{4-}$ clusters by using M062X, PBE0, B3LYP, X3LYP functionals. The average E-E distances and deviations from experiments (in parentheses) are displayed. I-IV denotes different E-E bonds assigned in Fig. S1.

d (E-E, Å)	Exp.	M062X	PBE0	B3LYP	X3LYP
$[Ge_9]^{4-}$	Ref.[1]				
I	2.589	2.601 (0.5%)	2.584 (-0.2%)	2.622 (1.3%)	2.618 (1.1%)
II	2.804	2.827 (0.8%)	2.825 (0.7%)	2.892 (3.1%)	2.885 (2.9%)
III	2.623	2.614 (-0.3%)	2.597 (-1.0%)	2.636 (0.5%)	2.632 (0.3%)
IV	2.537	2.625 (3.5%)	2.612 (3.0%)	2.652 (4.5%)	2.652 (4.5%)
$[Sn_9]^{4-}$	Ref.[2]				
I	2.954	2.982 (0.9%)	2.958 (0.1%)	3.004 (1.7%)	2.999 (1.5%)
II	3.178	3.227 (1.5%)	3.222 (1.4%)	3.295 (3.7%)	3.292 (3.6%)
III	3.012	3.006 (1.7%)	2.981 (0.8%)	3.026 (2.4%)	3.022 (2.2%)
IV	2.956	3.004 (-0.3%)	2.985 (0.9%)	3.038 (0.9%)	3.037 (0.8%)
$[Pb_9]^{4-}$	Ref.[3]				
I	3.065	3.106 (1.3%)	3.090 (0.8%)	3.146 (2.6%)	3.146 (2.6%)
II	3.355	3.397 (1.3%)	3.377 (0.7%)	3.456 (3.0%)	3.448 (2.8%)
III	3.061	3.151 (2.9%)	3.128 (2.2%)	3.199 (4.5%)	3.181 (3.9%)
IV	3.095	3.143 (1.6%)	3.119 (0.8%)	3.173 (2.5%)	3.171 (2.5%)

The negative sign indicates bond distance value is smaller than experiments.

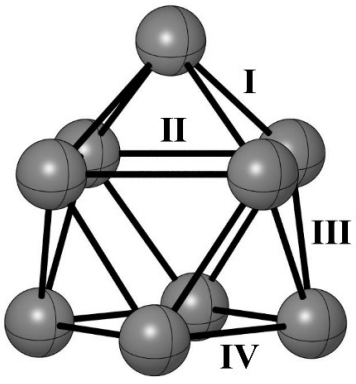

Fig. S1. The structure model for $[E_9]^{4-}$ (E = Ge, Sn, Pb) clusters and the E-E bonds are divided into four groups I, II, III and IV.

To determine the spin multiplicity of $[TM@E_9]^{n-}$ clusters, we calculated the energy difference between singlet and triplet states which termed ΔE_{S-T} ($\Delta E_{S-T} = E_{triplet} - E_{singlet}$) as shown in Table S2. The positive value demonstrated the spin multiplicity are all singlet.

Table S2 The ΔE_{S-T} (in eV) of $[TM@E_9]^{n-}$ (TM = Co, Ni, Cu; E = Ge, Sn, Pb) clusters.

Cluster	$[Co@E_9]^{5-}$	$[Ni@E_9]^{4-}$	$[Cu@E_9]^{3-}$
E = Ge	0.97	1.43	1.15
E = Sn	0.70	1.52	1.32
E = Pb	1.36	1.49	1.25

Table S3. The theoretical and experimental geometric information of $[TM@E_9]^{n-}$ clusters. The distance of E-E and TM-E (in Å) with average values (in parentheses) as well as the symmetry are displayed. h corresponds to the height of triangle prism (in Å). d represents the diagonal distance of square undersurface (in Å). α is bottom torsion dihedral (in degree).

Structure	E-E distance	TM-E distance	h_1	h_2	h_3	d_2/d_1	α	Sym.
$[Co@Ge_9]^{5-}$*	2.704-3.524 (2.797)	2.351-2.365 (2.355)	3.524	3.431	3.432	1.154	20.216	ca. D_{3h}
$[Co@Ge_9]^{5-}$[4]	2.683-3.483 (2.801)	2.331-2.374 (2.358)	3.524	3.431	3.432	1.123	18.472	ca. D_{3h}
$[Co@Sn_9]^{5-}$*	3.003-3.775 (3.107)	2.595-2.653 (2.615)	3.802	3.753	3.775	1.203	21.875	ca. D_{3h}
$[Co@Sn_9]^{5-}$[5]	2.955-3.555 (3.095)	2.581-2.680 (2.616)	4.220	3.555	3.441	1.020	3.712	ca. C_{4v}
$[Co@Sn_9]^{5-}$[6]	2.927-3.626 (3.080)	2.561-2.683 (2.603)	4.099	3.626	3.487	1.077	8.367	ca. C_{2v}
$[Ni@Sn_9]^{4-}$*	2.995-3.421 (3.104)	2.585-2.751 (2.627)	4.286	3.416	3.421	1.011	1.474	ca. C_{4v}
$[Ni@Sn_9]^{4-}$[7]	2.953-3.436 (3.060)	2.521-2.738 (2.588)	4.023	3.436	3.341	1.092	7.392	ca. C_{2v}
$[Ni@Sn_9]^{4-}$[5]	2.951-3.942 (3.140)	2.564-2.704 (2.622)	3.323	3.905	3.942	1.443	33.785	ca. C_{4v}
$[Cu@Sn_9]^{3-}$*	3.063-3.818 (3.159)	2.633-2.721 (2.661)	3.908	3.814	3.818	1.196	19.647	ca. D_{3h}
$[Cu@Sn_9]^{3-}$[8]	3.023-3.820 (3.139)	2.610-2.700 (2.645)	3.936	3.757	3.820	1.174	17.981	ca. D_{3h}
$[Cu@Pb_9]^{3-}$*	3.151-3.646 (3.267)	2.727-2.922 (2.767)	4.473	3.646	3.646	1.038	4.783	ca. C_{4v}
$[Cu@Pb_9]^{3-}$[8]	3.132-3.964 (3.257)	2.707-2.802 (2.745)	4.094	3.873	3.964	1.167	17.820	ca. D_{3h}

*the current theoretical work

Table S4. The energy difference of $[E_9]^{4-}$ and $[TM@E_9]^{n-}$ clusters with symmetry restriction.

Structure	Sym.	Restriction	ΔE (eV)
$[Ge_9]^{4-}$	C_{4v}	D_{3h}	0.024
$[Co@Ge_9]^{5-}$	D_{3h}	C_{4v}	0.031
$[Ni@Ge_9]^{4-}$	D_{3h}	C_{4v}	0.022
$[Cu@Ge_9]^{3-}$	D_{3h}	C_{4v}	0.017
$[Sn_9]^{4-}$	C_{4v}	D_{3h}	0.042
$[Co@Sn_9]^{5-}$	D_{3h}	C_{4v}	0.015
$[Ni@Sn_9]^{4-}$	C_{4v}	D_{3h}	0.003
$[Cu@Sn_9]^{3-}$	D_{3h}	C_{4v}	0.000
$[Pb_9]^{4-}$	C_{4v}	D_{3h}	0.043
$[Co@Pb_9]^{5-}$	C_{4v}	D_{3h}	0.006
$[Ni@Pb_9]^{4-}$	C_{4v}	D_{3h}	0.009
$[Cu@Pb_9]^{3-}$	C_{4v}	D_{3h}	0.012

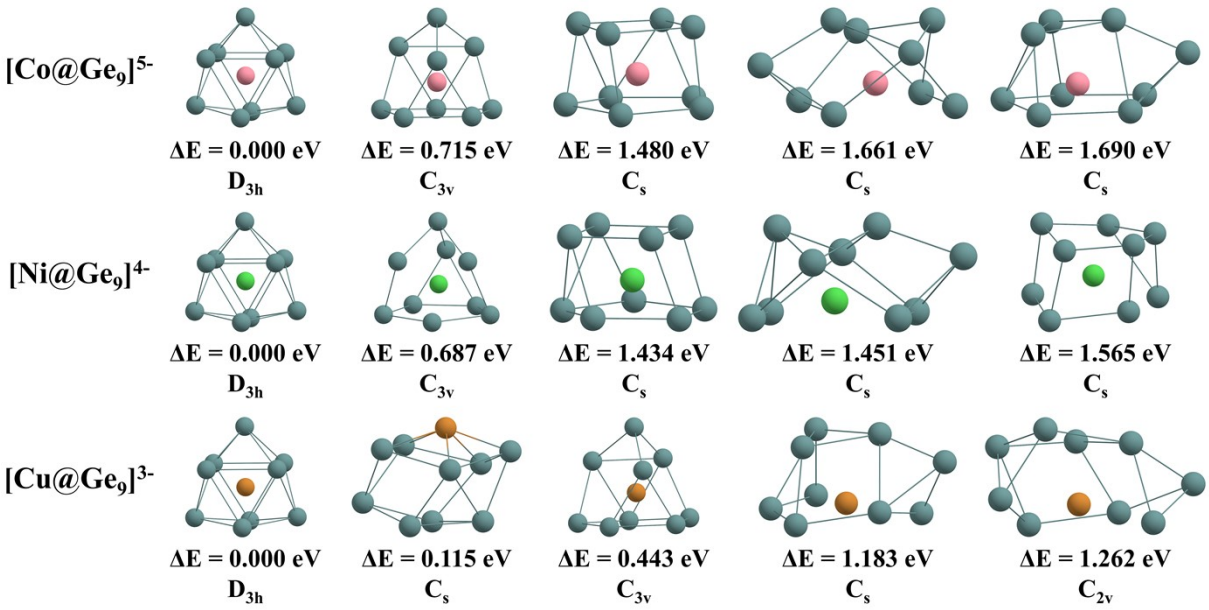

Fig. S2 The structural searching results of $[TM@Ge_9]^{n-}$ (TM = Co, Ni, Cu) clusters.

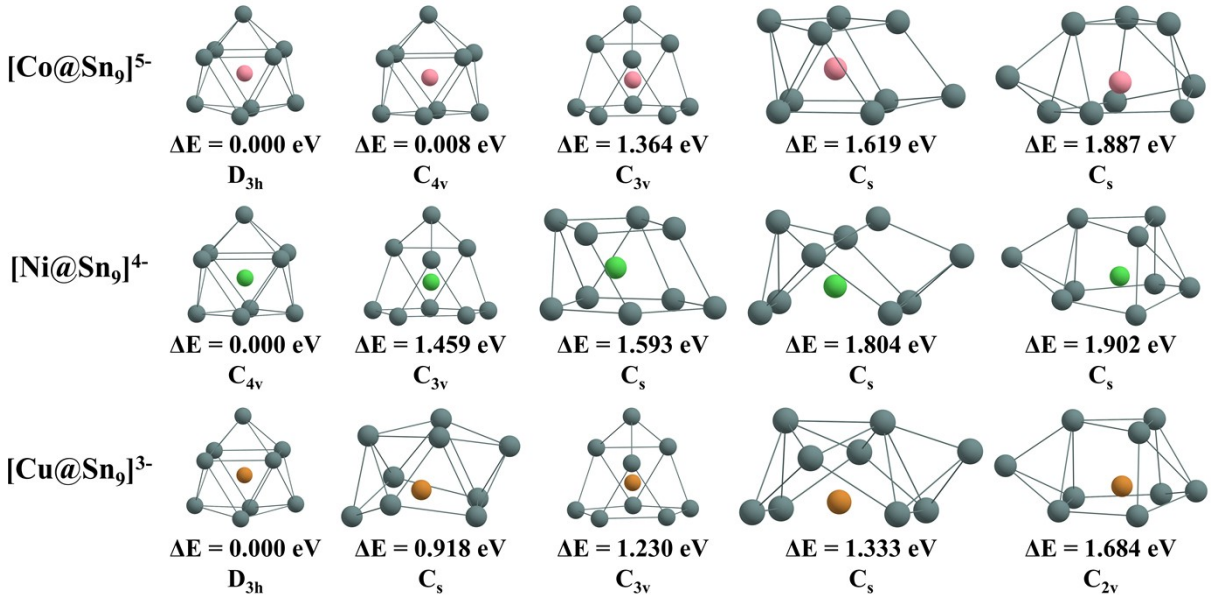

Fig. S3 The structural searching results of $[TM@Sn_9]^{n-}$ (TM = Co, Ni, Cu) clusters.

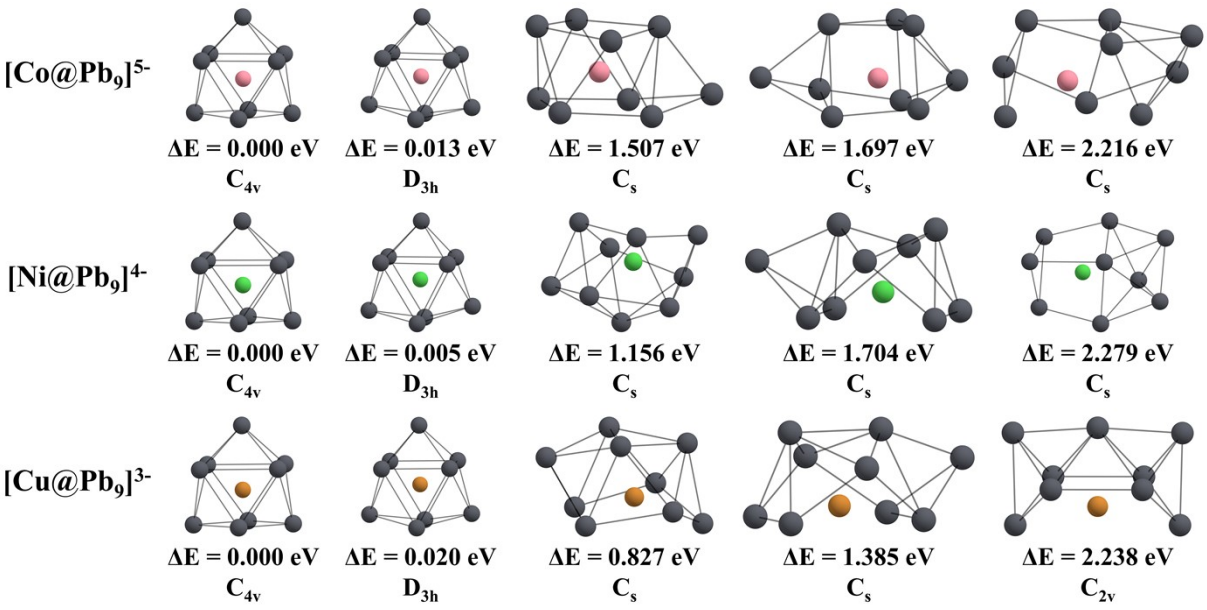

Fig. S4 The structural searching results of $[TM@Pb_9]^{n-}$ (TM = Co, Ni, Cu) clusters.

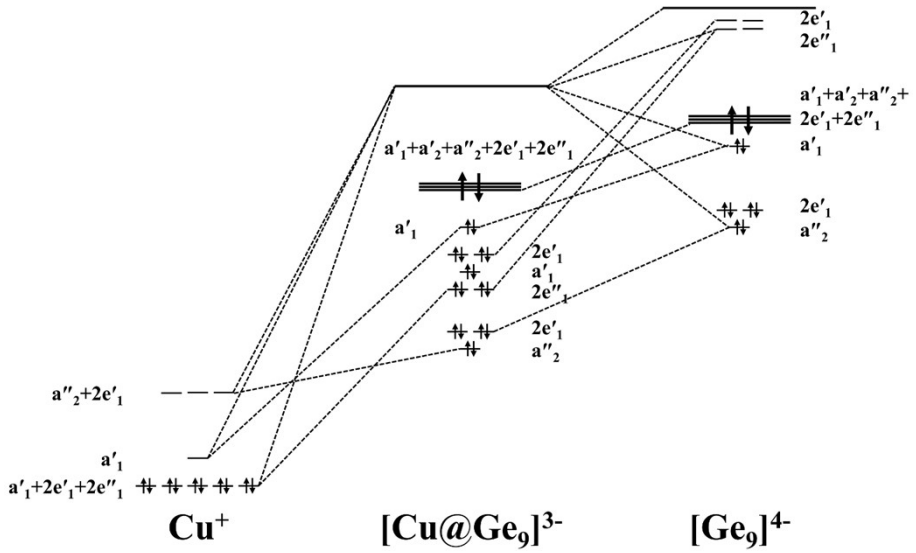

Fig. S5 The MO correlation diagram of valence orbitals of Cu with $[Ge_9]^{4-}$ in constructing $[Cu@Ge_9]^{3-}$ clusters.

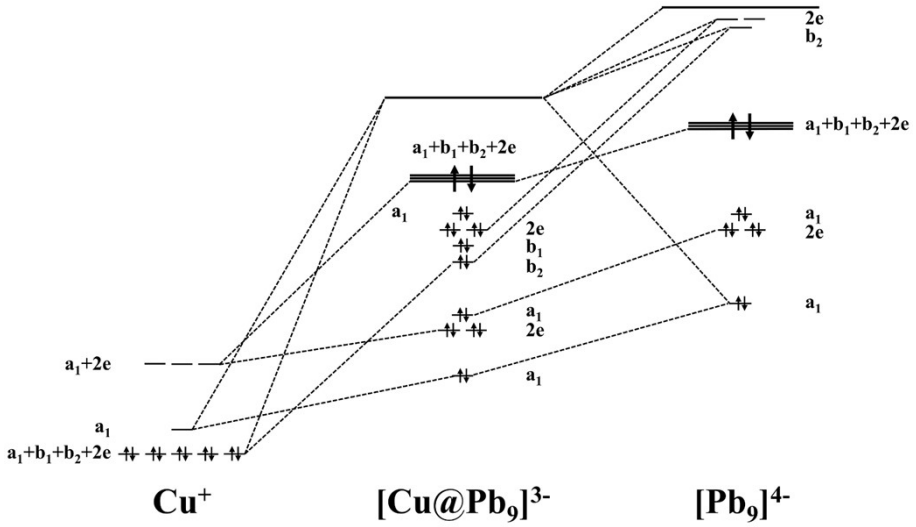

Fig. S6 The MO correlation diagram of valence orbitals of Cu with $[Pb_9]^{4-}$ in constructing $[Cu@Pb_9]^{3-}$ clusters.

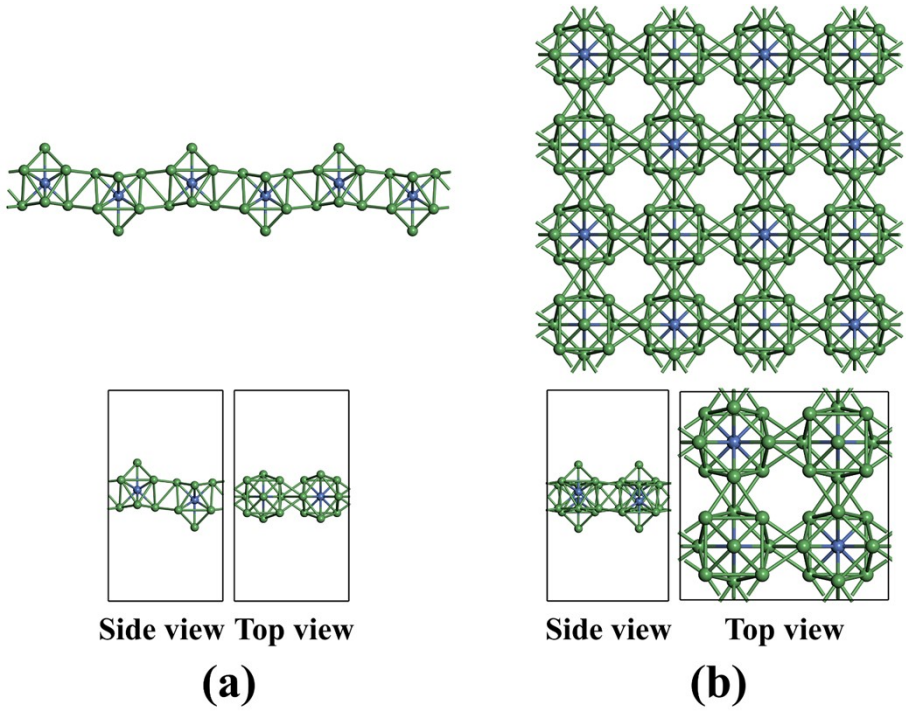

Fig. S7 The sketch maps for [Ni@Ge_9]-based (a) 1D-chain and (b) 2D-sheet nanostructures with corresponding optimized unit cell below.

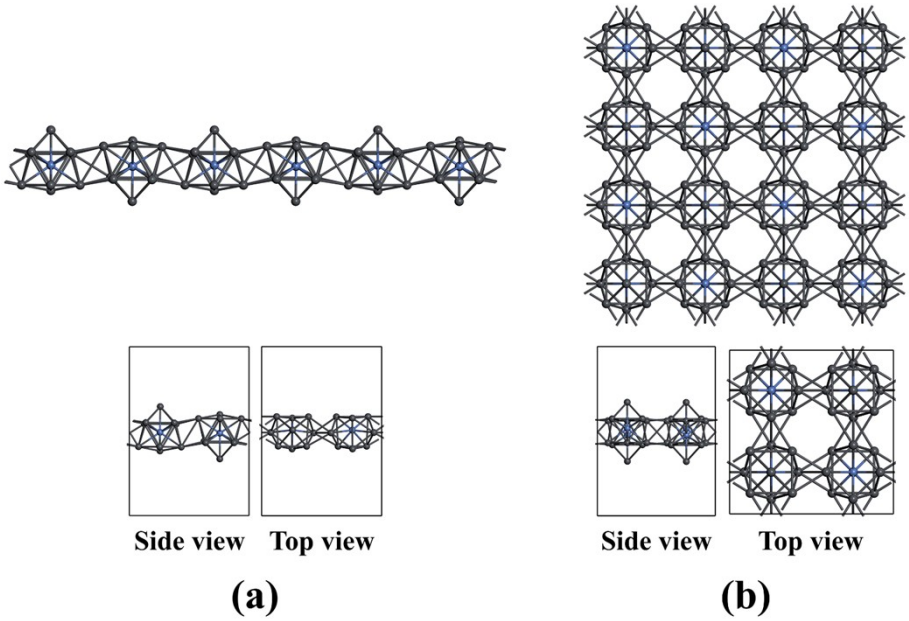

Fig. S8 The sketch maps for [Ni@Pb_9]-based (a) 1D-chain and (b) 2D-sheet nanostructures with corresponding optimized unit cell below.

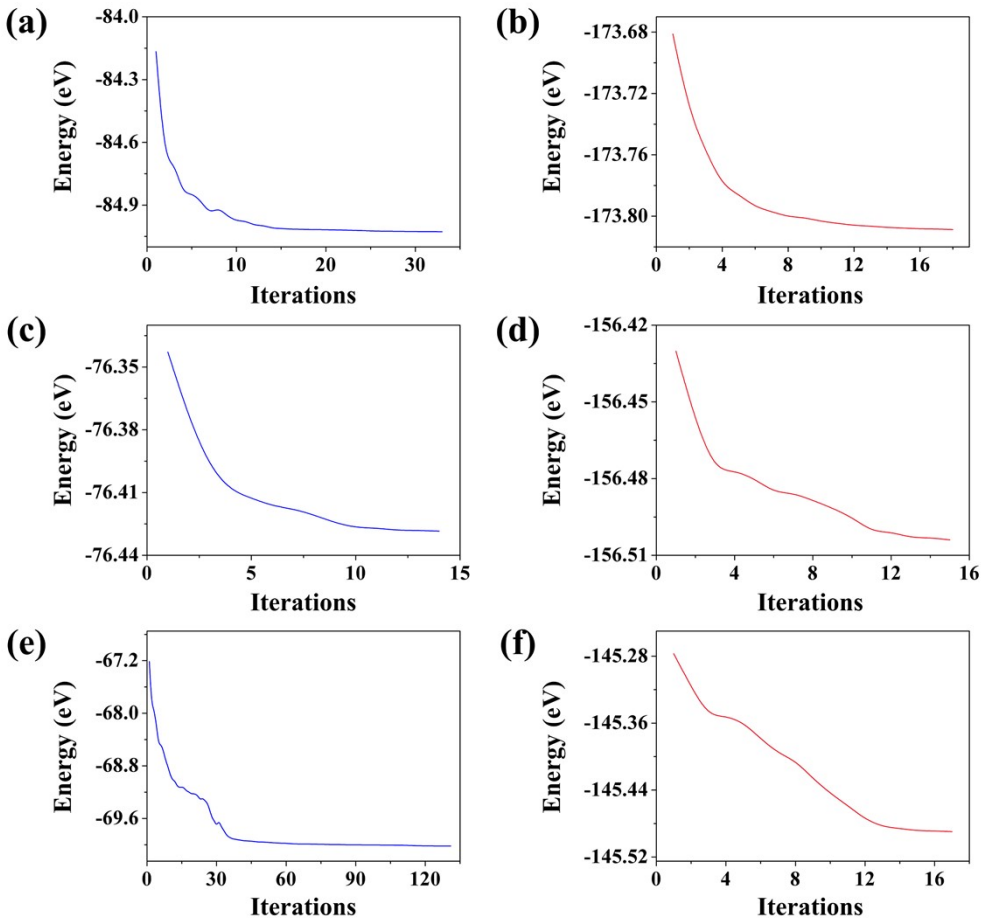

Fig. S9 The energy curves of TM@E_9 (E = Ge, Sn, Pb) nanostructures during the geometry optimization. (a), (b) corresponds to Ni@Ge_9-1D and Ni@Ge_9-2D. (c), (d) corresponds to Ni@Sn_9-1D and Ni@Sn_9-2D. (e), (f) corresponds to Ni@Pb_9-1D and Ni@Pb_9-2D.

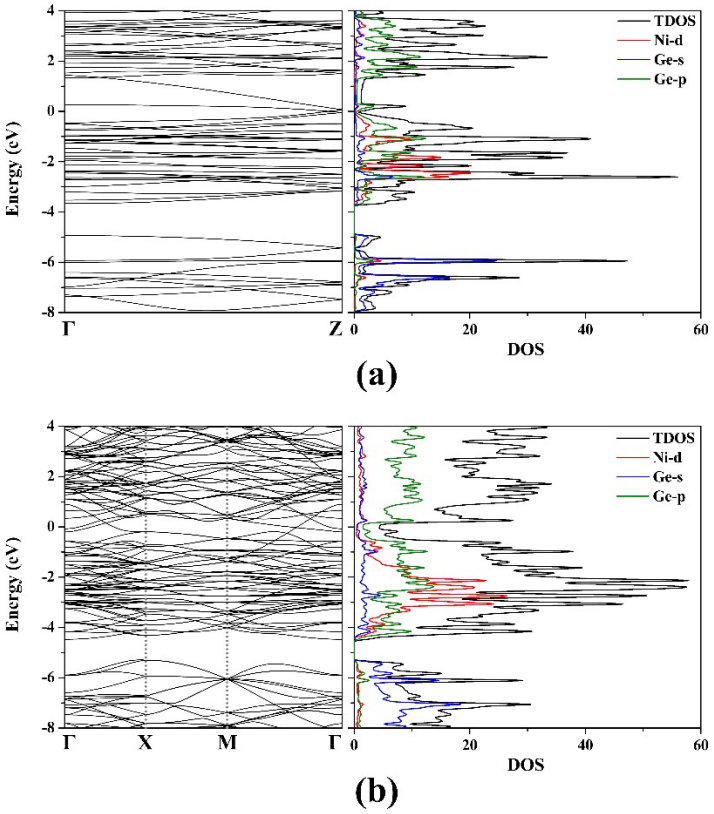

Fig. S10 The band structure and density of states for (a) [Ni@Ge_9]-chain and (b) [Ni@Ge_9]-sheet.

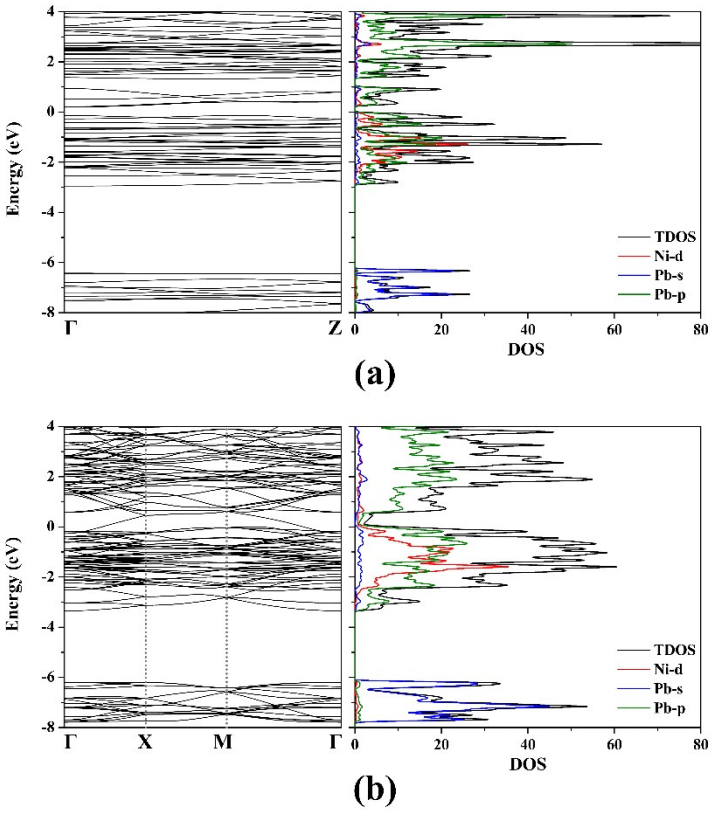

Fig. S11 The band structure and density of states for (a) [Ni@Pb_9]-chain and (b) [Ni@Pb_9]-sheet.

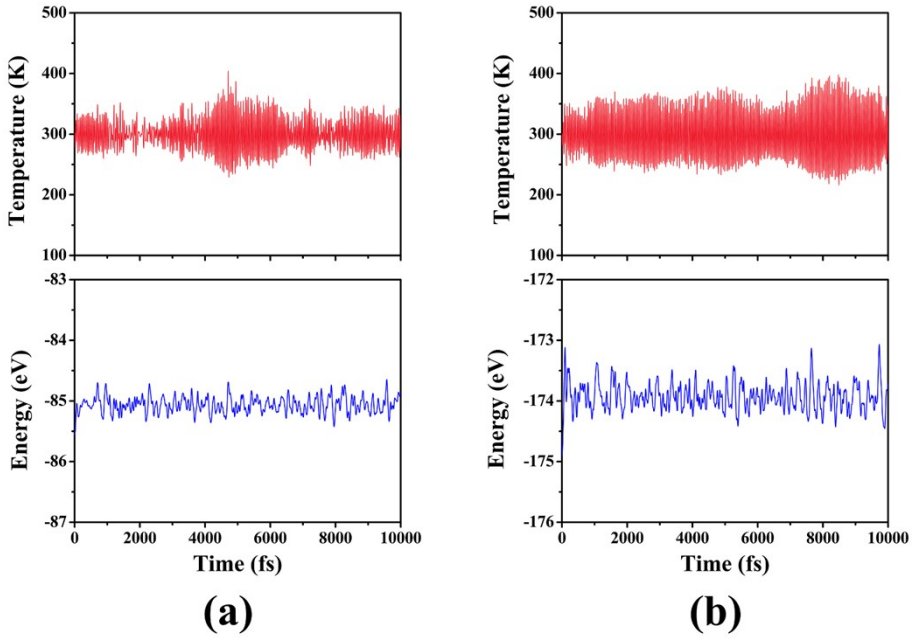

Fig. S12 The variation of temperature and energy with simulation time for [$NiGe_9$]-based (a) 1D-chain and (b) 2D-sheet materials.

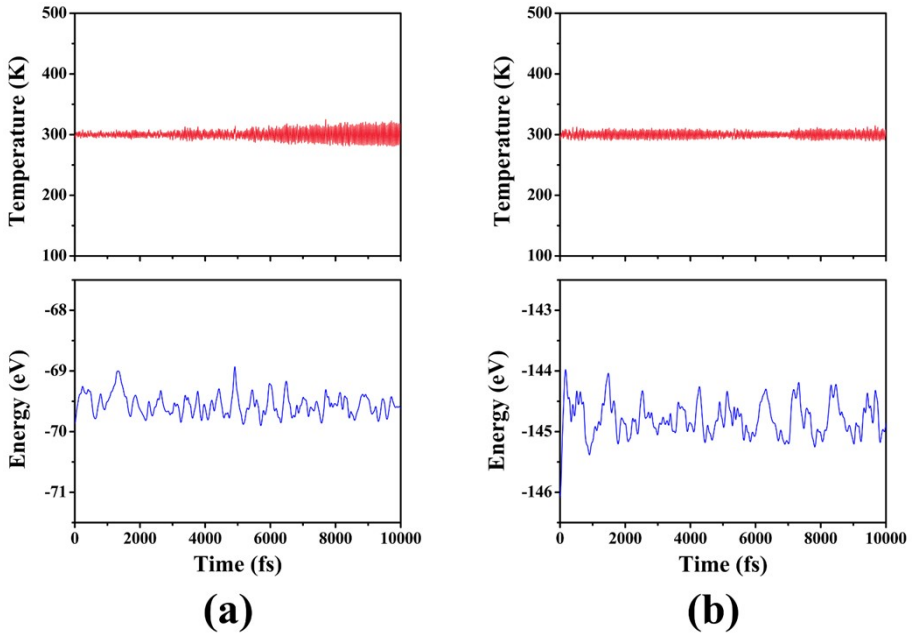

Fig. S13 The variation of temperature and energy with simulation time for [$NiPb_9$]-based (a) 1D-chain and (b) 2D-sheet materials.

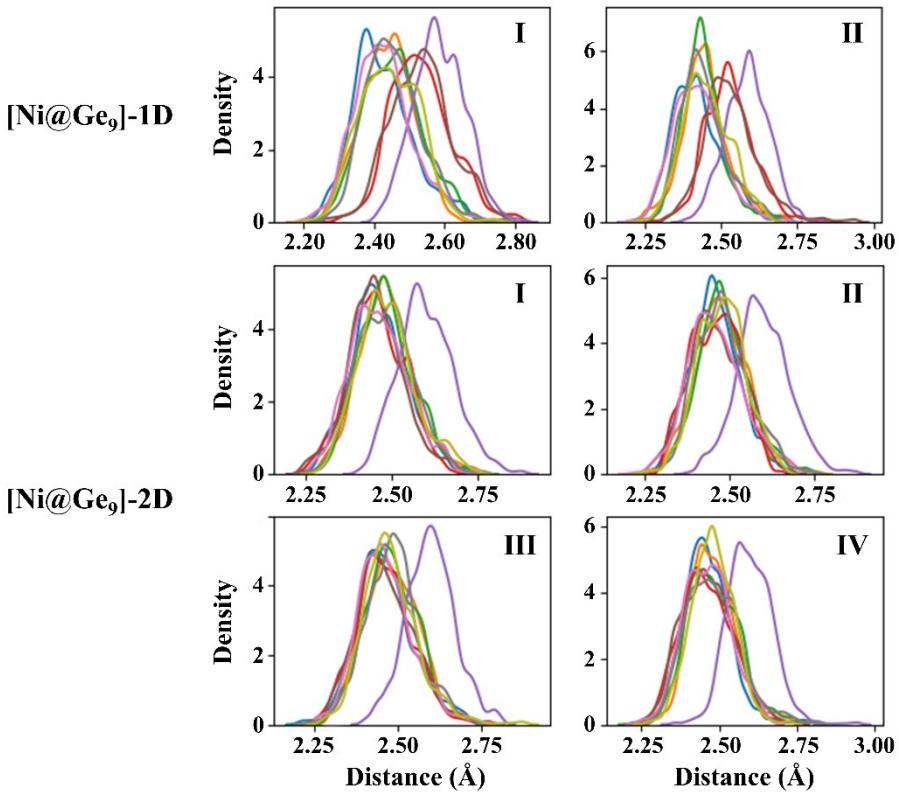

Fig. S14 The KDE maps of TM-E bond distance of every [Ni@Ge_9] units in 1D and 2D nanostructures. I-IV are represented the different units.

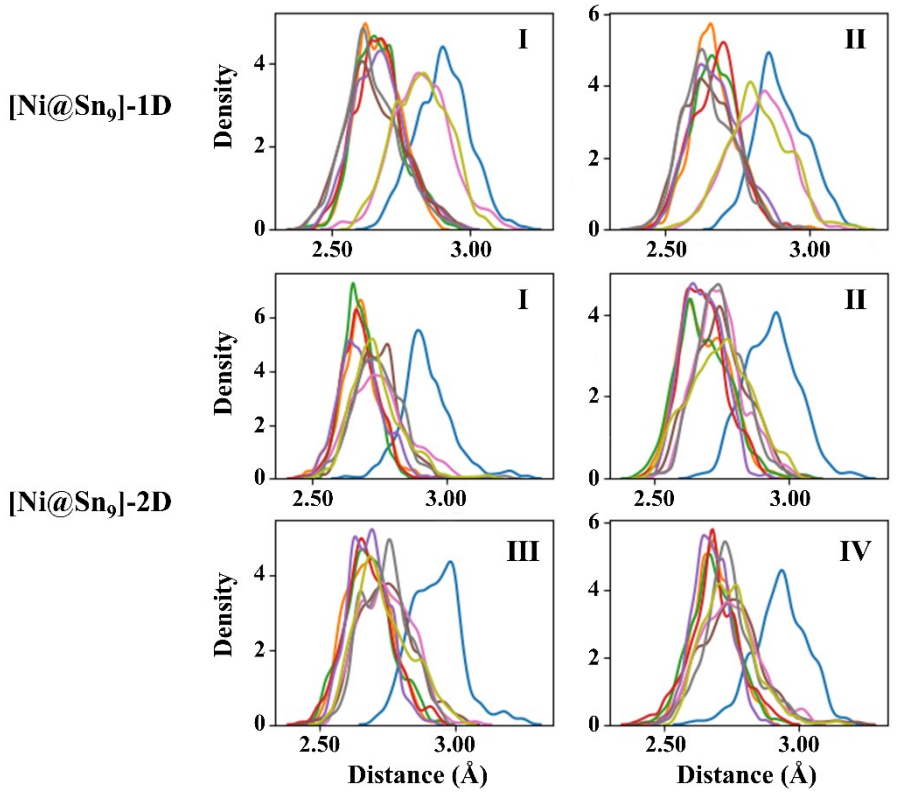

Fig. S15 The KDE maps of TM-E bond distance of every [Ni@Sn_9] units in 1D and 2D nanostructures. I-IV are represented the different units.

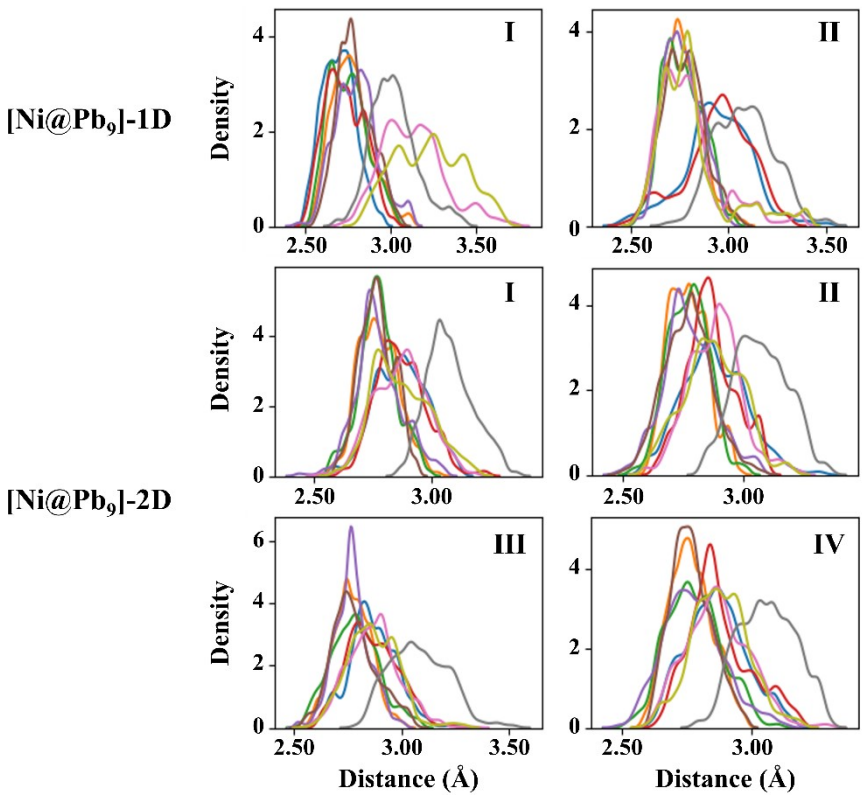

Fig. S16 The KDE maps of TM-E bond distance of every [Ni@Pb_9] units in 1D and 2D nanostructures. I-IV are represented the different units.

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Cartesian coordinates of optimized structures

$[TM@E_9]^{n-}$ cluster

PBE0/def2-TZVPPD, Singlet

$[Co@Ge_9]^{5-}$

Ge	1.76283600	-0.04328600	-1.56439600
Ge	0.00243200	-2.06702600	-1.14660200
Ge	0.00221400	1.99946300	-1.25973400
Ge	-1.76140000	-0.04367600	-1.56691200
Ge	-1.71632100	-1.37092000	0.83242400
Ge	1.71603400	-1.36803200	0.83715400
Ge	-1.71548000	1.41561000	0.75598800
Ge	1.71543900	1.41271400	0.76074800
Ge	-0.00535400	0.06538500	2.35709400
Co	-0.00047500	-0.00027600	-0.00683100

$[Ni@Ge_9]^{4-}$

Ge	1.76389300	0.00027600	1.56781400
Ge	1.71665100	-1.39221600	-0.79780300
Ge	1.71541400	1.39155400	-0.80080500
Ge	0.00208200	-2.05959900	1.21375200
Ge	- 0.00427400	-0.00338800	-2.38657200
Ge	0.00323400	2.05989300	1.21208100
Ge	-1.75963400	0.00243500	1.57160700
Ge	-1.72117500	-1.39119900	-0.79158500
Ge	-1.71634600	1.39262800	-0.79480000
Ni	0.00017800	-0.00044000	0.00721300

$[Cu@Ge_9]^{3-}$

Ge	-1.85064100	0.00849200	-1.54169700
Ge	0.00191900	2.08597300	-1.24927900
Ge	-0.00087200	-2.07423500	-1.26827000
Ge	1.85174800	0.00609400	-1.54026400
Ge	1.71256500	1.41944300	0.81193000
Ge	-1.71348600	1.41940900	0.80984300
Ge	1.71019100	-1.42837100	0.79848100
Ge	-1.71069800	-1.42786800	0.79885200
Ge	-0.00060000	-0.00953800	2.41466200
Cu	-0.00013900	0.00066300	-0.03780100

$[Co@Sn_9]^{5-}$

Sn	0.01726800	-2.58832000	-0.57499300
Sn	1.89492100	-1.19425600	1.30913400
Sn	-1.89531500	-0.55189600	-1.68779600
Sn	1.87981600	-0.52241000	-1.71261500
Sn	1.89040100	1.74911600	0.36748400
Sn	0.01102700	0.81517000	2.52069200
Sn	-0.02889100	1.79186100	-1.94845600
Sn	-1.85795900	-1.22217700	1.33507400
Sn	-1.91104300	1.72197800	0.39169700
Co	-0.00041600	0.00172800	-0.00040900

$[Ni@Sn_9]^{4-}$

Sn	0.01385900	-0.00007200	2.69990300
Sn	1.58340400	1.81003900	0.89716500
Sn	1.83546300	-1.55467000	0.89888400
Sn	-1.57637600	-1.80545100	0.91593900
Sn	-1.82318000	1.55643400	0.91492600
Sn	-0.16808000	2.15971100	-1.56137800
Sn	2.12849500	0.15447200	-1.59990800
Sn	0.15217700	-2.16108000	-1.55996200
Sn	-2.14592100	-0.15945700	-1.57714800
Ni	0.00028400	0.00013000	-0.05075300

$[Cu@Sn_9]^{3-}$

Sn	-1.95229300	-0.15179300	-1.77658300
Sn	-1.90891200	1.64268400	0.76157300
Sn	-1.90861700	-1.48662300	1.03231200
Sn	1.95521700	-0.15508600	-1.77318600
Sn	1.90869500	1.64057400	0.76616600
Sn	1.90581000	-1.48763200	1.03583000
Sn	-0.00054400	-2.44625000	-1.17148000
Sn	-0.00314700	0.23384000	2.70244700
Sn	0.00381000	2.21020900	-1.57212600
Cu	-0.00003500	0.00013100	-0.00854000

$[Co@Pb_9]^{5-}$

Pb	-2.19490800	1.66085800	-0.00391400
Pb	-1.77814300	-0.97094100	-1.71501800
Pb	-1.78091100	-0.96475100	1.71530400
Pb	2.14450900	1.72479400	-0.00165500

Pb	1.80787100	-0.91900300	-1.71289400
Pb	1.80701100	-0.91265800	1.71690800
Pb	-0.02433700	1.58805200	2.25861100
Pb	0.04081000	-2.80103700	0.00493700
Pb	-0.02174800	1.58304100	-2.26219800
Co	-0.00046300	0.03536600	-0.00024300

$[Ni@Pb_9]^{4-}$

Pb	-2.19143800	1.69388000	-0.01042700
Pb	-1.79693100	-0.95359300	-1.71496600
Pb	-1.79707100	-0.93179000	1.72667500
Pb	2.19074900	1.69469600	-0.01077300
Pb	1.79703300	-0.95313500	-1.71510200
Pb	1.79772800	-0.93132500	1.72623100
Pb	-0.00001700	1.60576400	2.27343400
Pb	0.00033600	-2.82075800	0.01774700
Pb	-0.00037600	1.57812800	-2.29267400
Ni	-0.00003900	0.05310000	-0.00042400

$[Cu@Pb_9]^{3-}$

Pb	2.23601900	-0.00150600	-1.70163300
Pb	1.82380700	1.74521400	0.94909400
Pb	1.82265400	-1.74532000	0.95076500
Pb	-2.23654700	-0.00012600	-1.70055200
Pb	-1.82239000	1.74574600	0.95048700
Pb	-1.82324000	-1.74385600	0.95220600
Pb	-0.00147900	-2.32195400	-1.60302200
Pb	0.00119500	0.00145100	2.83765300
Pb	-0.00008800	2.32033800	-1.60529000
Cu	0.00019800	0.00003700	-0.08400400

The primitive cells of $[Ni@E_9]$-based nanostructures

$[Ni@Ge_9]$-1D-chain

Ni	9.456399918	10.080599785	8.112112045
Ni	10.408200264	10.080399513	2.678422928
Ge	11.121200562	10.074000359	9.791574478
Ge	8.495800018	8.527400017	9.651800156
Ge	8.510000229	11.638000488	9.654735565
Ge	10.843800545	7.971400261	8.108851433
Ge	6.874799728	10.090199471	8.118308067
Ge	10.862999916	12.178400040	8.110264778
Ge	11.113800049	10.075199127	6.424171925
Ge	8.489000320	8.535400391	6.566011429
Ge	8.504199982	11.632599831	6.563729286
Ge	8.750800133	10.079000473	4.361798286
Ge	11.367198944	11.632200241	4.221045971
Ge	11.371200562	8.527200699	4.217894077
Ge	9.004600525	12.176199913	2.675488472
Ge	12.992600441	10.081600189	2.681140423
Ge	9.009799957	7.981400013	2.675597191
Ge	8.761600494	10.078599930	0.982439876
Ge	11.371400833	11.627799988	1.129713535
Ge	11.374799728	8.532199860	1.131561279

$[Ni@Ge_9]$-2D-sheet

Ni	8.717920303	8.714815140	10.546799660
Ni	2.963089943	8.713319778	9.658599854
Ni	2.966079950	2.961709976	10.543600082
Ni	8.714010239	2.958489895	9.677199364
Ge	8.714585304	6.795464993	9.000999451
Ge	7.148974895	7.148399830	11.566800117
Ge	10.277665138	7.147365570	11.573400497
Ge	6.802364826	8.714124680	8.994199753
Ge	8.713550568	8.709295273	13.134399414
Ge	10.631634712	8.709870338	8.996000290
Ge	8.717920303	10.629335403	9.001600266
Ge	7.152310371	10.276974678	11.573400497
Ge	10.281919479	10.276169777	11.575399399
Ge	2.959985018	10.627955437	11.210000992
Ge	1.397019982	10.276974678	8.635600090
Ge	4.528699875	10.276515007	8.637400627
Ge	1.050524950	8.709870338	11.213399887
Ge	2.963320017	8.709064484	7.074399948
Ge	4.878759861	8.717689514	11.212799072
Ge	2.967344999	6.799489975	11.213599205
Ge	1.400699973	7.144145012	8.642200470
Ge	4.530885220	7.148055077	8.643599510
Ge	2.965849876	4.875770092	8.991000175
Ge	4.530310154	4.524445057	11.565599442
Ge	1.402885079	4.526285172	11.571999550
Ge	4.882784843	2.956764936	8.998600006
Ge	2.967344999	2.962860107	13.133600235
Ge	1.047995090	2.963204861	9.000800133
Ge	2.961479902	1.046270013	8.993800163
Ge	4.527550220	1.394719958	11.571799278
Ge	1.400240064	1.399090052	11.573800087
Ge	8.718034744	1.046959996	11.232999802

Ge	10.282150269	1.395869970	8.654399872
Ge	7.149205208	1.392189980	8.656799316
Ge	10.629449844	2.963320017	11.229599953
Ge	8.710445404	2.956535101	7.090600014
Ge	6.802364826	2.956880093	11.234199524
Ge	8.713089943	4.874390125	11.230400085
Ge	10.275135040	4.523869991	8.653600693
Ge	7.150469780	4.523525238	8.657199860

[Ni@Sn_9]-1D-chain

Ni	10.362998960	10.114999780	9.232109070
Ni	9.401999480	10.112400060	3.069976331
Sn	13.288600920	10.210800180	9.239378932
Sn	11.330399520	11.853199960	10.948412896
Sn	11.343999860	11.853599540	7.520980364
Sn	11.479599000	8.426799780	7.548828125
Sn	11.466799740	8.431400300	10.925986295
Sn	8.562800400	10.060000420	11.094919199
Sn	8.759799960	12.462999340	9.222990987
Sn	8.577199940	10.055399900	7.355129241
Sn	8.944000240	7.657199860	9.230260849
Sn	6.479799740	10.200599680	3.062460180
Sn	8.430200580	11.849800100	1.351947909
Sn	8.417799940	11.848000520	4.783569335
Sn	8.295999520	8.419799800	4.753011221
Sn	8.308400160	8.422399520	1.379425524
Sn	11.206599240	10.070600500	1.208275681
Sn	10.996399880	12.470799440	3.076876637
Sn	11.189600000	10.065399160	4.945847038
Sn	10.839600560	7.666800020	3.071578497

[Ni@Sn_9]-2D-sheet

Ni	9.951292033	9.866183284	10.515999800
Ni	3.352900272	9.868690490	9.613599780
Ni	3.353032356	3.272145754	10.510400780
Ni	9.949576380	3.272673364	9.653800020
Sn	9.948653217	9.867502210	13.441200260
Sn	11.674981123	11.594358438	11.607600220
Sn	8.224964140	11.594885824	11.608400340
Sn	8.219553950	8.145396227	11.606999400
Sn	11.674057961	8.140250204	11.607799540
Sn	12.105671883	9.868426322	8.825200080
Sn	9.948256490	12.032966608	8.836200720
Sn	7.787411692	9.875551229	8.827799800
Sn	9.942187305	7.710615153	8.831600180
Sn	3.349865442	9.868557931	6.690999980
Sn	1.621030329	11.594094271	8.525199900
Sn	5.073950296	11.598976138	8.525599480
Sn	5.078436374	8.143022542	8.523799900
Sn	1.624197124	8.142625802	8.525400160
Sn	1.191394684	9.865391730	11.302000040
Sn	3.349205735	12.028612139	11.301399240
Sn	5.511106967	9.870537752	11.303199760
Sn	3.354483841	7.707580086	11.301399240
Sn	3.348018167	3.271090032	13.435200700
Sn	1.622745639	1.547005178	11.600199700
Sn	5.074873920	1.544102313	11.601200100
Sn	5.075797558	4.997682093	11.604199400
Sn	1.626440282	5.000057216	11.603000640
Sn	1.185984494	3.277687790	8.830200200
Sn	3.344851253	1.115390306	8.819199560
Sn	5.510711190	3.272805448	8.828399660
Sn	3.351580857	5.432067865	8.821200380
Sn	9.946146011	3.272673364	6.726200100
Sn	11.673001289	1.548324698	8.561400420
Sn	8.219553950	1.548456663	8.563200000
Sn	8.219422341	4.998605730	8.559599880
Sn	11.670495033	5.002696031	8.560000420
Sn	12.108971593	3.276368138	11.337800020
Sn	9.949180603	1.114070773	11.339999200
Sn	7.785696026	3.273069378	11.338399880
Sn	9.945090289	5.434179308	11.336400980

[Ni@Pb_9]-1D-chain

Pb	11.967200280	11.547000880	3.453567509
Pb	8.778599740	11.727000240	1.600406050
Pb	8.784999840	11.702199940	5.338890073
Pb	11.498999600	7.906399720	3.435574049
Pb	8.627399440	8.219599720	1.769287348
Pb	8.632400520	8.206800460	5.135438914
Pb	11.496800420	9.806400300	5.976019859
Pb	6.718999860	10.122400280	3.458809377
Pb	11.483600620	9.843199720	0.909720836
Pb	7.660799980	11.551400180	10.540209764
Pb	10.868999480	11.727399820	12.392520908
Pb	10.833599100	11.710599900	8.636185644
Pb	8.141400340	7.903199680	10.569820406
Pb	11.022399900	8.228599540	12.213863376

Pb	10.98740006	8.209000580	8.851962096
Pb	8.123600000	9.804800040	8.019314764
Pb	12.912399300	10.135601040	10.504648208
Pb	8.166600220	9.850399980	13.083913809
Ni	9.765800480	10.121799460	3.457251078
Ni	9.866000180	10.139599800	10.532275202

[Ni@Pb_9]-2D-sheet

Pb	3.556716676	12.807077409	11.237200740
Pb	1.776756764	12.308743479	8.400199900
Pb	5.334309102	12.299412728	8.400600440
Pb	3.541396137	8.230155938	11.239999780
Pb	1.770907047	8.738378521	8.398400300
Pb	5.326231009	8.732250207	8.400199900
Pb	5.838631149	10.507614132	11.233200080
Pb	3.555602544	10.521680830	6.442599780
Pb	1.260317563	10.526695248	11.233600620
Pb	10.507892602	12.799835200	8.602399820
Pb	12.279217716	12.296905519	11.451799400
Pb	8.722500803	12.296209329	11.437999720
Pb	10.520288464	8.234056474	8.600799560
Pb	12.286599161	8.739213946	11.451400760
Pb	8.731832502	8.731971737	11.432800300
Pb	8.221382142	10.511374471	8.605999940
Pb	10.494522094	10.517781255	13.399800300
Pb	12.809863088	10.519591327	8.619999880
Pb	10.49229335	1.264217263	11.203999520
Pb	12.27935600	1.765475397	8.371000280
Pb	8.721804613	1.775363924	8.365799900
Pb	10.514299386	5.840999122	11.205600740
Pb	12.288967134	5.325674054	8.369199760
Pb	8.730718606	5.338209151	8.370200160
Pb	8.217342371	3.561034208	11.207400320
Pb	10.511513707	3.553652527	6.414999960
Pb	12.788692469	3.541117666	11.210199360
Pb	3.548638819	1.270624047	8.623999600
Pb	1.759068613	1.767703648	11.459399220
Pb	5.322331434	1.775363924	11.463199620
Pb	3.540699961	5.843226914	8.633199700
Pb	1.752522469	5.327484613	11.465400700
Pb	5.314531796	5.330409054	11.472999580
Pb	5.828464025	3.561452150	8.622799880
Pb	3.534014706	3.547106744	13.420200340
Pb	1.256557112	3.550588363	8.618800160
Ni	3.548220877	10.515692713	9.536200520
Ni	10.506917956	10.516806609	10.302800180
Ni	10.504828452	3.550866847	9.508200640
Ni	3.540143020	3.553513528	10.324600220

The low-energy isomers of [TM@E_9]$^{n-}$ clusters

[Co@Ge_9]$^{5-}$

ΔE = 0.000 eV

Ge	-0.006282000	0.904221000	2.177489000
Ge	1.760606000	-0.601934000	-1.447870000
Ge	0.001343000	1.414992000	-1.887449000
Ge	0.003933000	-2.339038000	-0.326998000
Ge	1.722177000	-0.973980000	1.269006000
Ge	-1.722348000	-0.978054000	1.262031000
Ge	-1.753690000	-0.608218000	-1.452305000
Ge	1.713071000	1.594471000	0.207514000
Ge	-1.718615000	1.589945000	0.202226000
Co	-0.000232000	-0.002850000	-0.004320000

ΔE = 0.715 eV

Co	0.077300000	-0.000320000	0.000657000
Ge	-0.323731000	0.107527000	-2.441715000
Ge	-1.709613000	-0.068239000	1.663431000
Ge	2.016015000	1.243793000	0.821314000
Ge	2.008156000	-1.339459000	0.671148000
Ge	-0.333818000	-2.168741000	1.126715000
Ge	-1.701741000	1.482618000	-0.771635000
Ge	-0.322752000	2.060990000	1.314442000
Ge	2.013298000	0.083032000	-1.488197000
Ge	-1.711036000	-1.401250000	-0.896058000

ΔE = 1.480 eV

Co	-0.002596000	0.037247000	-0.118136000
Ge	-1.381372000	0.937653000	1.568149000
Ge	-1.334153000	2.048329000	-0.711856000
Ge	-0.017368000	-1.901628000	-1.445545000
Ge	1.464421000	0.900957000	1.524677000
Ge	-2.159180000	-0.371884000	-1.130878000
Ge	2.155980000	-0.437763000	-1.104804000
Ge	1.364682000	-1.616086000	1.111560000
Ge	1.365623000	1.990624000	-0.779012000
Ge	-1.456441000	-1.581629000	1.067387000

ΔE = 1.661 eV

Co	-0.258683000	0.000169000	-0.446882000
Ge	1.591153000	1.324368000	-1.089643000
Ge	3.397067000	-0.000910000	0.205055000
Ge	-2.001415000	-0.000696000	1.347170000
Ge	1.591963000	-1.322150000	-1.090654000
Ge	-2.260744000	-1.276747000	-0.991473000
Ge	1.128002000	-0.000256000	1.448857000
Ge	-0.484201000	2.068522000	0.770339000
Ge	-0.483379000	-2.068849000	0.768969000
Ge	-2.260182000	1.276575000	-0.991562000

ΔE = 1.690 eV

Co	-0.243976000	-0.001827000	-0.336813000
Ge	-1.174830000	2.101013000	-0.949620000
Ge	-1.170515000	1.410984000	1.466938000
Ge	1.559374000	1.336387000	-1.015102000
Ge	-2.631344000	-0.032550000	-0.638640000
Ge	-1.125785000	-2.141681000	-0.900611000
Ge	-1.203004000	-1.365654000	1.494587000
Ge	3.301820000	-0.038652000	0.386320000
Ge	1.086716000	-0.013666000	1.563476000
Ge	1.563423000	-1.254639000	-1.123162000

$[Ni@Ge_9]^{4-}$

ΔE = 0.000 eV

Ni	0.001205000	-0.000256000	0.005679000
Ge	1.727194000	1.409615000	-0.748408000
Ge	-1.736324000	-1.342205000	-0.841989000
Ge	-0.005744000	0.088723000	-2.383830000
Ge	1.708492000	-1.373097000	-0.852423000
Ge	-1.712636000	1.429092000	-0.739884000
Ge	-0.012720000	-2.107766000	1.127632000
Ge	-1.747822000	-0.050847000	1.581277000
Ge	1.760934000	-0.069475000	1.568348000
Ge	0.017571000	2.016184000	1.284307000

ΔE = 0.687 eV

Ni	0.092721000	0.000218000	0.000531000
Ge	-0.348049000	2.167473000	-1.264486000
Ge	-1.667494000	-1.428076000	0.823645000
Ge	1.985549000	-0.013434000	1.501118000
Ge	1.992435000	-1.278061000	-0.765541000
Ge	-0.327136000	-2.179291000	-1.248648000
Ge	-1.674696000	1.428056000	0.815382000
Ge	-0.345552000	0.003359000	2.506376000
Ge	1.979416000	1.314332000	-0.729737000
Ge	-1.675605000	-0.014549000	-1.638573000

ΔE = 1.434 eV

Ni	-0.001509000	0.080916000	-0.095033000
Ge	-1.524462000	0.777933000	1.556674000
Ge	-1.406240000	2.081883000	-0.630643000
Ge	0.015420000	-1.830188000	-1.530710000
Ge	1.513126000	0.799018000	1.555554000
Ge	-2.152006000	-0.335406000	-1.087400000
Ge	2.144381000	-0.266948000	-1.113923000
Ge	1.436141000	-1.702549000	0.948987000
Ge	1.344523000	2.131071000	-0.601144000
Ge	-1.369562000	-1.725616000	0.985759000

ΔE = 1.451 eV

Ni	-0.318591000	-0.000738000	-0.598371000
Ge	1.654727000	1.304538000	-1.112109000
Ge	3.344938000	-0.000914000	0.374343000
Ge	-1.756708000	-0.000059000	1.487423000
Ge	1.654554000	-1.303213000	-1.114903000
Ge	-2.395049000	-1.275474000	-0.834735000
Ge	1.019245000	0.000182000	1.360350000
Ge	-0.425051000	2.161193000	0.600169000
Ge	-0.424464000	-2.161393000	0.599858000
Ge	-2.393423000	1.275787000	-0.836822000

ΔE = 1.565 eV

Ni	-0.388025000	-0.275585000	0.337827000
Ge	1.424104000	0.775510000	1.380231000
Ge	-0.735422000	-2.239619000	-0.834155000
Ge	-1.772821000	0.018313000	-1.647033000
Ge	0.082271000	1.695165000	-1.097753000
Ge	1.696580000	-1.301636000	-0.674857000
Ge	-2.734446000	0.056809000	0.729732000
Ge	0.885172000	-1.829348000	1.636412000
Ge	2.486192000	1.170880000	-0.975166000
Ge	-0.992110000	1.895063000	1.186990000

$[Cu@Ge_9]^{3-}$

ΔE = 0.000 eV

Cu	0.000047000	-0.000166000	-0.039367000
Ge	-1.709011000	1.427068000	0.802719000
Ge	0.001873000	2.078558000	-1.261920000
Ge	1.708082000	-1.425895000	0.807023000
Ge	-1.711049000	-1.422649000	0.806407000
Ge	-0.001443000	-2.081322000	-1.257567000
Ge	-1.853148000	-0.000769000	-1.540168000
Ge	1.710172000	1.425451000	0.803230000
Ge	-0.000374000	0.002884000	2.414172000
Ge	1.854857000	-0.003175000	-1.538219000

ΔE = 0.115 eV

Cu	0.694592000	0.000008000	1.618447000
Ge	1.104882000	-2.025191000	0.183093000
Ge	-0.836769000	1.447643000	-1.413561000
Ge	-0.836858000	-1.448643000	-1.413179000
Ge	-1.277362000	1.396192000	1.330840000
Ge	-2.711982000	-0.000341000	-0.311429000
Ge	1.329667000	0.000419000	-1.755362000
Ge	-1.276360000	-1.395463000	1.332198000
Ge	2.770525000	-0.000080000	0.397263000
Ge	1.104785000	2.025458000	0.183421000

ΔE = 0.443 eV

Cu	-0.118900000	0.001099000	-0.036396000
Ge	-2.019622000	1.299330000	-0.766239000
Ge	0.353729000	-2.217063000	-1.263181000
Ge	1.648659000	1.455489000	0.805938000
Ge	-1.986748000	0.014906000	1.515713000
Ge	1.652061000	-1.432424000	0.838871000
Ge	0.357056000	2.183478000	-1.319816000
Ge	0.372720000	0.030124000	2.551519000
Ge	-2.019680000	-1.313129000	-0.739826000
Ge	1.749578000	-0.02107000	-1.589994000

ΔE = 1.183 eV

Cu	0.279096000	0.205001000	0.734405000
Ge	-1.108725000	0.691375000	-1.343466000
Ge	2.590388000	-0.531823000	0.549859000
Ge	-1.639332000	-1.347314000	0.628690000
Ge	1.437214000	1.330752000	-1.435991000
Ge	-1.835556000	1.093057000	1.472556000
Ge	-3.368090000	0.365869000	-0.393801000
Ge	0.838067000	-2.395979000	0.579902000
Ge	2.167805000	1.872204000	0.909575000
Ge	0.665297000	-1.263923000	-1.632879000

ΔE = 1.262 eV

Cu	-0.062400000	1.235542000	0.003925000
Ge	1.322965000	-0.437527000	1.367588000
Ge	-0.276508000	-1.964382000	-0.003187000
Ge	1.321173000	-0.432553000	-1.366807000
Ge	2.286699000	1.658168000	0.002455000
Ge	-1.414909000	0.138966000	-1.875199000
Ge	-2.512290000	1.516427000	0.003084000
Ge	-2.720747000	-1.141822000	-0.003612000
Ge	-1.415701000	0.129291000	1.875134000
Ge	3.465869000	-0.586277000	-0.003013000

$[Co@Sn_9]^{5-}$

ΔE = 0.000 eV

Sn	1.940048000	-1.741666000	-0.136704000
Sn	-1.882162000	0.990593000	-1.480351000
Sn	-0.009343000	-1.195386000	-2.360480000
Sn	1.852017000	1.009510000	-1.503290000
Sn	-1.857340000	0.776163000	1.629094000
Sn	1.871383000	0.793592000	1.607952000
Sn	-0.011112000	2.644282000	0.182764000
Sn	0.022141000	-1.516902000	2.170532000
Sn	-1.926256000	-1.755755000	-0.109892000
Co	0.001154000	-0.008207000	0.000692000

ΔE = 0.008 eV

Co	-0.000215000	-0.001156000	-0.036224000
Sn	2.159197000	0.296478000	-1.506076000
Sn	0.363668000	-2.128802000	-1.530929000
Sn	-2.062446000	-0.332510000	-1.625983000
Sn	1.901902000	-1.415244000	0.979258000
Sn	-0.267495000	2.094366000	-1.597768000
Sn	-1.461275000	-1.915869000	0.879219000
Sn	1.404196000	1.934083000	0.923447000
Sn	-1.955877000	1.438162000	0.832709000
Sn	-0.081755000	0.029962000	2.665685000

ΔE = 1.364 eV

Co	0.098177000	0.000585000	0.001212000
Sn	-0.358160000	-0.945420000	2.607079000
Sn	-1.917748000	0.624460000	-1.719143000

Sn	2.256028000	-1.076610000	-1.293959000
Sn	2.256096000	1.661708000	-0.286503000
Sn	-0.359765000	2.731658000	-0.484980000
Sn	-1.910218000	-1.809295000	0.319395000
Sn	-0.359036000	-1.784481000	-2.123353000
Sn	2.256911000	-0.582047000	1.578868000
Sn	-1.917125000	1.179711000	1.401943000

ΔE = 1.619 eV

Co	0.291487000	-0.000056000	-0.066580000
Sn	-1.395849000	0.000190000	1.809025000
Sn	1.667444000	1.533514000	-1.578420000
Sn	1.666400000	-1.535054000	-1.577765000
Sn	-1.327793000	-1.683613000	-0.991431000
Sn	-1.327052000	1.684511000	-0.991024000
Sn	2.673969000	-0.000277000	1.015218000
Sn	0.741431000	2.233735000	1.256439000
Sn	-3.596502000	0.000141000	-0.163439000
Sn	0.740548000	-2.233117000	1.257351000

ΔE = 1.887 eV

Co	-0.270938000	-0.006908000	-0.277559000
Sn	-1.261793000	2.329974000	-1.153090000
Sn	-1.328400000	1.560155000	1.624195000
Sn	1.625853000	1.541837000	-1.008336000
Sn	-2.943330000	-0.001337000	-0.642624000
Sn	-1.250885000	-2.336800000	-1.141093000
Sn	-1.416852000	-1.531730000	1.631679000
Sn	3.796157000	-0.033861000	0.241318000
Sn	1.292490000	-0.075076000	1.755693000
Sn	1.633067000	-1.449430000	-1.157860000

$[Ni@Sn_9]^{4-}$

ΔE = 0.000 eV

Sn	-2.088377000	-0.353717000	1.616882000
Sn	-2.019163000	1.263728000	-0.962402000
Sn	0.443629000	-2.050525000	1.651455000
Sn	-0.433774000	2.197885000	1.460161000
Sn	2.014242000	-1.347764000	-0.849743000
Sn	-1.343334000	-2.032823000	-0.806505000
Sn	2.097927000	0.503529000	1.565027000
Sn	-0.008280000	-0.129491000	-2.696910000
Sn	1.336625000	1.947114000	-1.005014000
Ni	0.000902000	0.003685000	0.048303000

ΔE = 1.459 eV

Ni	0.114276000	-0.001265000	0.000976000
Sn	-0.383940000	-2.393687000	-1.578483000
Sn	-1.838669000	1.519976000	1.007307000
Sn	2.198887000	1.528766000	-0.723621000
Sn	2.208567000	-0.142759000	1.675132000
Sn	-0.368619000	-0.173583000	2.862344000
Sn	-1.848877000	0.107727000	-1.810402000
Sn	-0.382840000	2.566078000	-1.281746000
Sn	2.198604000	-1.388152000	-0.969999000
Sn	-1.847108000	-1.623659000	0.818922000

ΔE = 1.593 eV

Sn	2.688007000	-0.000904000	-0.947230000
Sn	-1.270869000	-1.850902000	0.920383000
Sn	-1.270742000	1.852002000	0.919404000
Sn	-1.462700000	-0.001318000	-1.838778000
Sn	0.704685000	-2.217281000	-1.316773000
Sn	1.604567000	1.529936000	1.620607000
Sn	-3.454871000	0.000268000	0.333513000
Sn	0.705318000	2.216065000	-1.319232000
Sn	1.605178000	-1.528121000	1.621698000
Ni	0.270402000	0.000457000	0.011442000

ΔE = 1.804 eV

Sn	-2.531102000	1.443529000	1.064202000
Sn	-2.063175000	0.001921000	-1.619411000
Sn	1.654994000	-1.471895000	1.284007000
Sn	3.771700000	-0.001959000	-0.258365000
Sn	-0.452527000	2.438325000	-0.766571000
Sn	1.165271000	-0.001227000	-1.561522000
Sn	-0.456042000	-2.437844000	-0.766316000
Sn	-2.536199000	-1.441693000	1.061778000
Sn	1.655936000	1.471872000	1.281817000
Ni	-0.372957000	-0.001838000	0.500681000

ΔE = 1.902 eV

Ni	-0.308492000	-0.007895000	-0.301506000
Sn	-1.313734000	2.374923000	-1.159643000
Sn	-1.222327000	1.614553000	1.624984000
Sn	1.563969000	1.628851000	-0.911790000
Sn	-2.913825000	-0.034125000	-0.596286000
Sn	-1.241770000	-2.422823000	-1.108454000

Sn	-1.349823000	-1.571572000	1.653975000
Sn	3.737746000	-0.089556000	0.178721000
Sn	1.317720000	-0.128517000	1.767868000
Sn	1.594800000	-1.367312000	-1.280532000

$[Cu@Sn_9]^{3-}$

ΔE = 0.000 eV

Sn	1.912754000	1.512222000	0.989037000
Sn	-0.003805000	-2.244669000	-1.523165000
Sn	0.001005000	-0.146341000	2.709799000
Sn	1.967103000	0.101350000	-1.770460000
Sn	1.886518000	-1.634128000	0.813342000
Sn	-1.892428000	-1.62819000	0.813976000
Sn	-1.966580000	0.107169000	-1.770692000
Sn	0.003905000	2.411387000	-1.242823000
Sn	-1.908419000	1.516832000	0.989811000
Cu	-0.000091000	0.005167000	-0.015215000

ΔE = 0.918 eV

Sn	0.789179000	1.599131000	-1.552080000
Sn	-1.376401000	-2.389740000	0.394381000
Sn	-1.828437000	-0.003880000	-1.773969000
Sn	-2.993057000	0.001858000	1.040369000
Sn	0.789454000	-1.601923000	-1.550377000
Sn	-1.377889000	2.390591000	0.389136000
Sn	1.529940000	1.543437000	1.574246000
Sn	1.529733000	-1.541272000	1.575439000
Sn	3.127406000	0.000810000	-0.420331000
Cu	-0.327463000	0.00706000	0.557220000

ΔE = 1.230 eV

Cu	0.134421000	-0.002025000	-0.000288000
Sn	-0.396706000	-0.374034000	-2.883523000
Sn	-1.851665000	0.231235000	1.813836000
Sn	2.219076000	1.569051000	0.669441000
Sn	2.228286000	-1.359858000	1.017972000
Sn	-0.388180000	-2.313985000	1.764047000
Sn	-1.854435000	1.449591000	-1.108544000
Sn	-0.400126000	2.684513000	1.120408000
Sn	2.222123000	-0.197990000	-1.693011000
Sn	-1.856337000	-1.687349000	-0.700458000

ΔE = 1.333 eV

Sn	-1.824170000	-1.480005000	-1.270052000
Sn	0.453311000	-2.474428000	0.599396000
Sn	1.931425000	-0.000363000	1.736816000
Sn	2.735408000	1.445634000	-0.917686000
Sn	-3.792044000	0.000484000	0.435528000
Sn	0.454188000	2.474385000	0.598926000
Sn	-1.119567000	0.000387000	1.477816000
Sn	-1.823502000	1.480074000	-1.270269000
Sn	2.734509000	-1.446117000	-0.918349000
Cu	0.431799000	-0.000091000	-0.814009000

ΔE = 1.684 eV

Cu	-0.358258000	0.000152000	-0.460844000
Sn	-1.310617000	2.478080000	-1.097502000
Sn	-1.244537000	1.602771000	1.662737000
Sn	1.601627000	1.532516000	-1.131336000
Sn	-2.952296000	-0.000025000	-0.578621000
Sn	-1.310990000	-2.478264000	-1.097289000
Sn	-1.242869000	-1.602815000	1.662722000
Sn	3.718315000	0.000274000	0.173421000
Sn	1.348137000	0.001433000	1.801902000
Sn	1.601020000	-1.534059000	-1.128745000

$[Co@Pb_9]^{5-}$

ΔE = 0.000 eV

Pb	-2.056309000	1.902542000	-0.104922000
Pb	0.389633000	1.912682000	1.795924000
Pb	0.633576000	1.981207000	-1.643838000
Pb	-2.019827000	-0.703388000	1.570174000
Pb	2.706708000	0.464096000	0.203853000
Pb	-1.770448000	-0.625435000	-1.870330000
Pb	1.341240000	-1.043281000	-2.179937000
Pb	-0.248650000	-2.742476000	-0.076142000
Pb	1.015118000	-1.137669000	2.304404000
Co	0.027210000	-0.025141000	0.002474000

ΔE = 0.013 eV

Pb	1.597987000	0.125930000	2.247880000
Pb	-0.858577000	-1.838802000	-1.704602000
Pb	-1.029320000	1.779876000	1.672898000
Pb	1.674583000	-0.018784000	-2.195095000
Pb	-0.917426000	-1.728852000	1.788397000
Pb	1.573119000	2.265708000	-0.046919000
Pb	1.716809000	-2.159204000	0.099954000
Pb	-2.801592000	-0.089977000	-0.043791000

Pb	-0.968904000	1.663682000	-1.818995000
Co	0.040455000	0.001282000	0.000825000

ΔE = 1.507 eV

Pb	-2.041808000	-1.846262000	0.009305000
Pb	-0.211363000	2.791543000	-0.120232000
Pb	-1.904223000	0.872470000	1.627246000
Pb	1.651184000	1.146977000	1.729647000
Pb	-1.799534000	0.732634000	-1.805434000
Pb	0.049377000	-1.501794000	2.319496000
Pb	0.193504000	-1.681639000	-2.185950000
Pb	2.299149000	-1.509199000	0.132922000
Pb	1.762746000	1.007344000	-1.707465000
Co	0.002941000	-0.036677000	0.001410000

ΔE = 1.697 eV

Pb	1.819884000	1.740904000	-1.129530000
Pb	-2.786965000	0.297163000	0.057501000
Pb	1.452491000	-2.090506000	1.066760000
Pb	1.475044000	-1.265601000	-1.961074000
Pb	-0.917241000	0.753710000	-2.368086000
Pb	-0.960720000	-0.555222000	2.407457000
Pb	-1.206841000	-2.275550000	-0.631224000
Pb	-0.671845000	2.477401000	0.661595000
Pb	1.783387000	0.919251000	1.896712000
Co	0.038897000	-0.004711000	-0.000334000

ΔE = 2.216 eV

Pb	-1.928092000	-1.116883000	-1.494987000
Pb	0.001962000	1.101796000	-2.546383000
Pb	1.928553000	-1.118814000	-1.493017000
Pb	-0.001591000	-2.757442000	0.335261000
Pb	-1.932320000	-0.729665000	1.711858000
Pb	-1.948725000	1.840416000	-0.221321000
Pb	-0.000369000	1.672706000	2.213893000
Pb	1.929757000	-0.731604000	1.713888000
Pb	1.950822000	1.838529000	-0.219183000
Co	0.000010000	0.002925000	-0.000030000

$[Ni@Pb_9]^{4-}$

ΔE = 0.000 eV

Pb	0.001915000	-0.200997000	2.810458000
Pb	0.272127000	2.352972000	-1.459144000
Pb	-1.973236000	-1.577502000	0.833140000
Pb	1.972205000	1.445385000	1.049392000
Pb	-0.271716000	-2.122764000	-1.778134000
Pb	2.203416000	-0.143956000	-1.680005000
Pb	1.552880000	-2.006635000	0.802601000
Pb	-2.205377000	0.383948000	-1.639804000
Pb	-1.552334000	1.868209000	1.080993000
Ni	0.000351000	0.003929000	-0.057102000

ΔE = 0.005 eV

Pb	0.045700000	-1.616900000	2.263923000
Pb	-1.748802000	0.938038000	1.770986000
Pb	-0.053263000	-1.591772000	-2.281936000
Pb	1.833457000	0.929300000	1.688889000
Pb	1.748543000	0.949979000	-1.761042000
Pb	0.005282000	2.821381000	0.020187000
Pb	2.195100000	-1.689671000	-0.056695000
Pb	-1.821280000	0.957854000	-1.685008000
Pb	-2.204583000	-1.679795000	0.040676000
Ni	-0.000447000	-0.053925000	0.000061000

ΔE = 1.156 eV

Pb	1.859229000	-1.029742000	1.617162000
Pb	1.876071000	-0.827159000	-1.714690000
Pb	-0.017070000	1.366139000	2.432840000
Pb	0.016350000	-2.806163000	-0.172304000
Pb	-2.108296000	1.754036000	0.099104000
Pb	-1.854421000	-0.846176000	-1.728532000
Pb	-1.860773000	-1.050712000	1.601653000
Pb	-0.000446000	1.651910000	-2.249208000
Pb	2.089530000	1.775521000	0.113603000
Ni	-0.000512000	0.036155000	0.001090000

ΔE = 1.704 eV

Pb	-0.883886000	-1.642169000	1.578655000
Pb	-1.467899000	-1.567846000	-1.661065000
Pb	1.933009000	0.001274000	1.832369000
Pb	-3.309843000	-0.001276000	0.312059000
Pb	1.454550000	2.430426000	-0.371823000
Pb	-1.470132000	1.566536000	-1.659577000
Pb	-0.885085000	1.641805000	1.579220000
Pb	3.076187000	0.001356000	-1.132669000
Pb	1.457927000	-2.430018000	-0.369710000
Ni	0.278717000	-0.000258000	-0.314705000

ΔE = 2.279 eV

Pb	1.469143000	1.566901000	-1.659989000
Pb	0.885322000	-1.641879000	1.578275000
Pb	1.467752000	-1.567194000	-1.660443000
Pb	0.884673000	1.641432000	1.579118000
Pb	3.310456000	-0.000026000	0.311273000
Pb	-1.456037000	2.430252000	-0.371593000
Pb	-3.077049000	0.000403000	-1.131491000
Pb	-1.932099000	0.000230000	1.833154000
Pb	-1.456696000	-2.430183000	-0.370858000
Ni	-0.279575000	0.000189000	-0.314658000

$[Cu@Pb_9]^{3-}$

ΔE = 0.000 eV

Pb	2.285358000	0.146088000	-1.642908000
Pb	-0.015926000	-0.009410000	2.838883000
Pb	1.662401000	1.883949000	0.967675000
Pb	-0.131833000	2.282559000	-1.648134000
Pb	-2.269584000	-0.135589000	-1.666051000
Pb	0.149942000	-2.272542000	-1.660160000
Pb	1.884897000	-1.668376000	0.957340000
Pb	-1.672682000	-1.892586000	0.937985000
Pb	-1.892444000	1.666063000	0.947960000
Cu	-0.000364000	-0.000441000	-0.092149000

ΔE = 0.020 eV

Pb	-0.177973000	-2.296496000	1.630111000
Pb	2.281442000	-0.203718000	1.639504000
Pb	-0.040859000	0.013066000	-2.838619000
Pb	-1.640527000	1.928889000	-0.920071000
Pb	1.929660000	1.607675000	-0.969037000
Pb	1.624090000	-1.908086000	-0.981885000
Pb	-2.243565000	0.185353000	1.694762000
Pb	-1.951950000	-1.604408000	-0.936538000
Pb	0.220228000	2.278312000	1.649052000
Cu	-0.001545000	-0.001661000	0.092521000

ΔE = 0.827 eV

Pb	1.989536000	-1.340791000	-1.313489000
Pb	-1.991876000	-0.467245000	1.816703000
Pb	1.991767000	-0.467254000	1.816786000
Pb	1.990505000	1.807324000	-0.503312000
Pb	-0.000053000	2.017685000	1.977053000
Pb	0.000090000	0.705184000	-2.735479000
Pb	-0.000027000	-2.721237000	0.758929000
Pb	-1.989436000	-1.340792000	-1.313632000
Pb	-1.990501000	1.807293000	-0.503438000
Cu	-0.000017000	-0.000469000	-0.000343000

ΔE = 1.385 eV

Pb	1.915743000	0.000286000	-1.829000000
Pb	-3.283950000	-0.000398000	-0.368042000
Pb	-0.855965000	-1.658561000	-1.596881000
Pb	1.468445000	2.467437000	0.381402000
Pb	-0.856110000	1.659214000	-1.595947000
Pb	-1.549728000	1.615881000	1.654420000
Pb	1.468501000	-2.467580000	0.381669000
Pb	-1.550743000	-1.615600000	1.653901000
Pb	3.124618000	-0.000605000	1.121344000
Cu	0.337015000	-0.000209000	0.557417000

ΔE = 2.238 eV

Pb	-1.551459000	1.615306000	-1.655026000
Pb	1.914624000	0.001618000	1.828710000
Pb	1.468738000	2.467135000	-0.381111000
Pb	3.124854000	0.000353000	-1.121312000
Pb	-0.857339000	1.659019000	1.596256000
Pb	-1.550086000	-1.616523000	-1.654128000
Pb	1.470614000	-2.467123000	-0.380320000
Pb	-0.856072000	-1.658635000	1.597170000
Pb	-3.283083000	-0.000984000	0.367786000
Cu	0.337074000	-0.000465000	-0.559931000