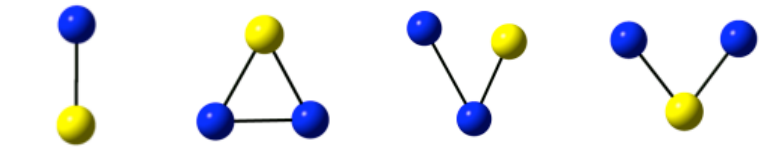
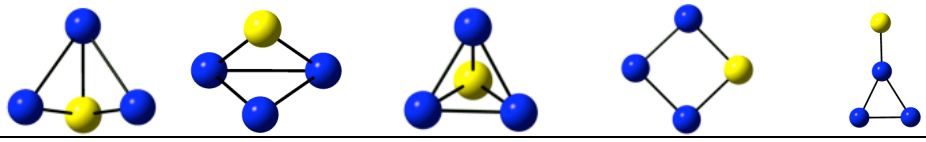
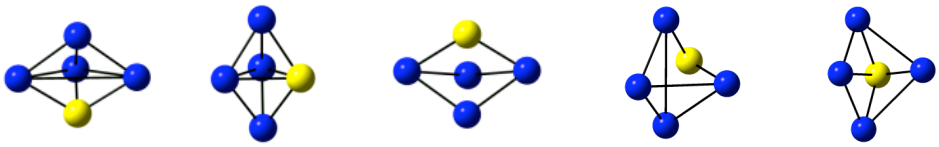
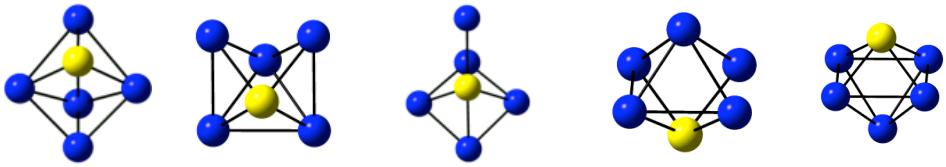
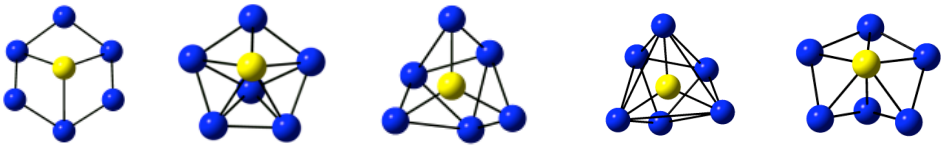
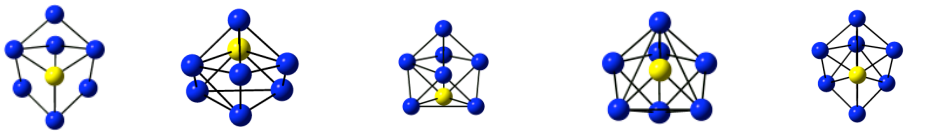
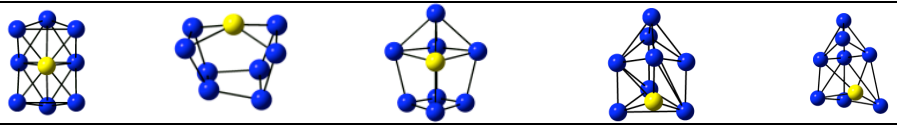
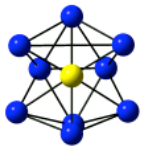
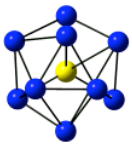
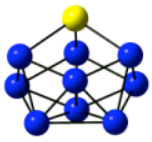
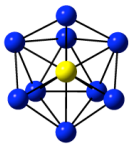
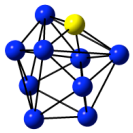
Electronic Supplementary Material (ESI) for RSC Advances.

Figure 1Sa. Optimized structures of Ge_n Mo (n=1-20) clusters with point group symmetry and relative energy (Kcal/mol) with respect to the ground state isomer in each size. Blue balls are Ge and yellow balls are Mo atoms.

n	Isomers				
1 & 2					
	C_V:GS	GS: C_{2V}	C_{2V}:△E =0.069	C_{2V} :△E=0.092	
3					
	C_{2V}:GS	C_{2V}:△E =0.04	C_1:△E=0.23	C_1:△E=1.46	C_1:△E=14.30
4					
	C_{2V}:GS	C_{2V}:△E =0.023	C_{2V}:△E =0.27	C_1:△E=1.46	C_1:△E=1.47
5					
	C_S:GS	C:△E =0.01	C_{2V}:△E=0.23	C_1:△E=0.38	C_1:△E=1.77
6					
	C_1:GS	C_1:△E=0.39	C_1:△E=0.46	C_1:△E=5.80	C_1:△E=6.45
7					
	C_1:GS	C_1:△E=0.006	C_1:△E=0.52	C_1:△E=0.53	C_1:△E=0.64
8					
	C_{2V}:GS	C_1:△E=0.01	C_{2V}:△E=0.56	C_1:△E=28.51	C_1:△E=37.57

9					
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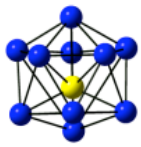
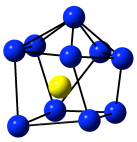
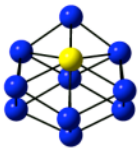
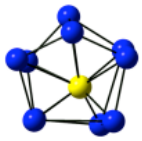
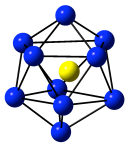
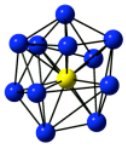
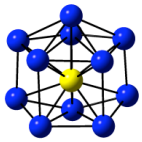
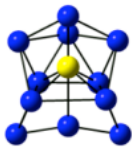
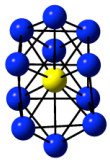
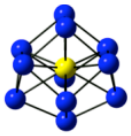
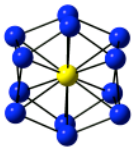
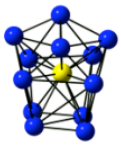
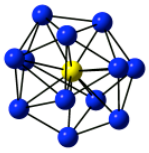
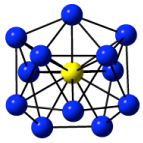
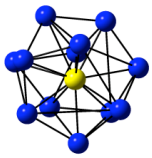
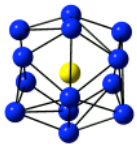
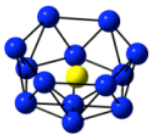
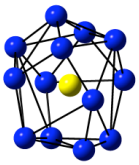
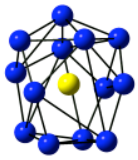
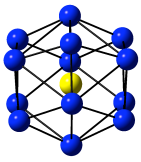
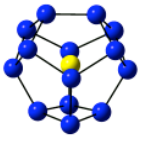
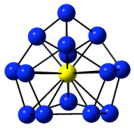
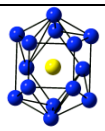
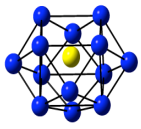
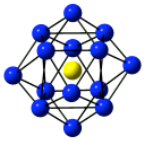
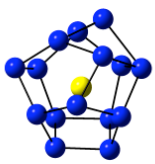
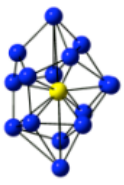
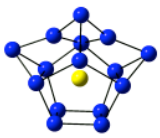
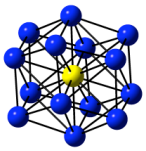
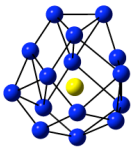
10					
	C_1:GS	C_2:△E=0.18	C_1:△E=0.18	C:△E=0.20	C_1:△E=0.24
11					
	C_S:GS	C:△E= 2.55	C:△E=5.30	C_1:△E= 7.89	C_1:△E=44.7
12					
	C_1:GS	C:△E=0.59	C:△E=0.66	C:△E=21.32	C_1:△E=23.52
13					
	C_S:GS	C_1:△E=7.29	C_1:△E=7.89	C_1:△E=16.89	C_1:△E=28.65
14					
	C_S:GS	C_1:△E=0.06	C_1:△E=7.29	C_1:△E=12.15	C_1:△E=16.8
15					
	C_1:GS	C:△E=10.8	C_2:△E=40.3	C_2:△E=54.19	C:△E=58.21

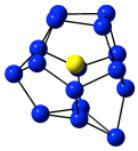
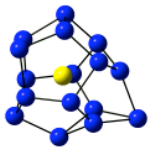
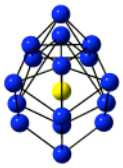
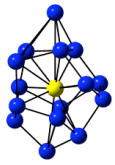
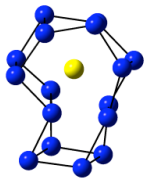
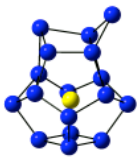
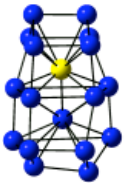
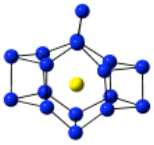
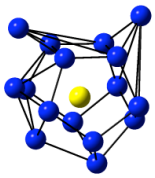
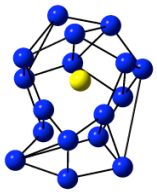
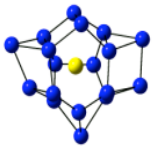
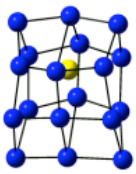
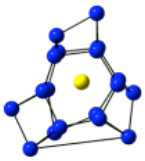
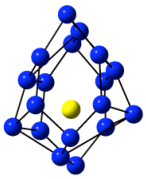
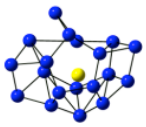
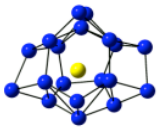
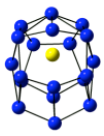
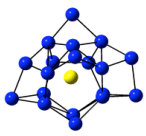
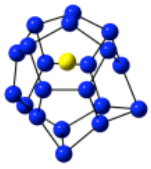
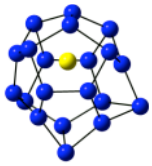
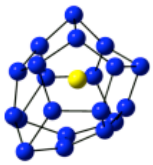
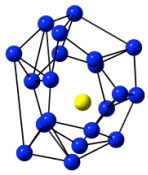
16					
	C_1:GS	C_1:△E=3.22	C_1:△E=14.8	C_1:△E=54.30	C_1:△E=57.95
17					
	C_1:GS	C_1:△E=0.91	C_S:△E=1.25	C_1:△E=72.20	C_1:△E=81.26
18					
	C_S:GS	C_1:△E=2.37	C:△E=63.1	C_1:△E=63.2	
19					
	C_1:GS	C_1:△E=0.23	C_1:△E=2.31	C_1:△E=60.36	
20					
	C_1:GS	C_1:△E=0.23	C_1:△E=1.84	C_1:△E=29.54	

Fig.1Sb. Different valence orbital's of $Mo@Ge_{12}$ in neutral and different charged state

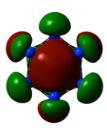
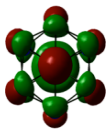
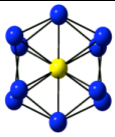
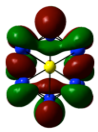
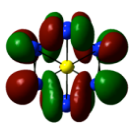
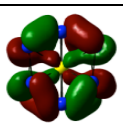
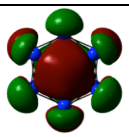
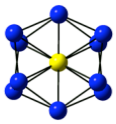
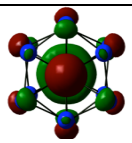
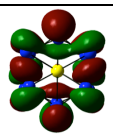
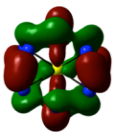
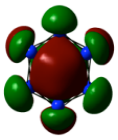
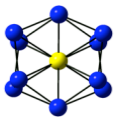
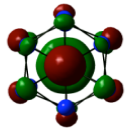
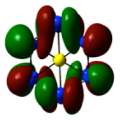
				
HOMO-1	**HOMO**	**$Ge_{12}Mo$ Anion**	**LUMO**	**LUMO+1**
				
HOMO-1	**HOMO**	**$Ge_{12}Mo$ Neutral**	**LUMO**	**LUMO+1**
				
HOMO-1	**HOMO**	**$Ge_{12}Mo$ Cation**	**LUMO**	**LUMO+1**

Fig. 1Sc. Onsite magnetic moment of low energy neutral and cationic isomers with the bond lengths and relative energies with respect to the ground state neutral cluster. Dip blue balls are Mo and pink balls are Ge. Onsite magnetc moment is written in green in terms of μ_B.

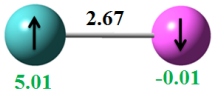
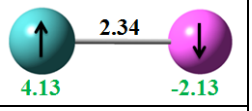
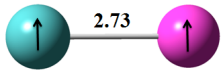
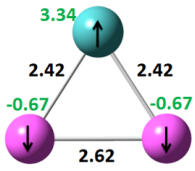
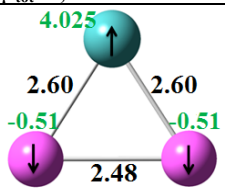
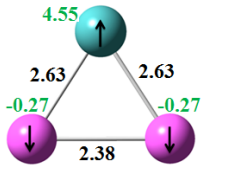
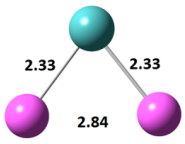
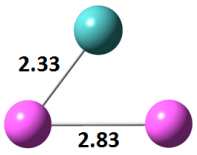
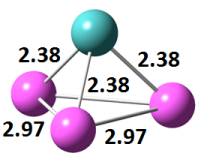
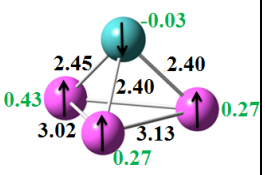
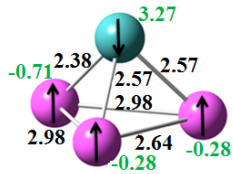
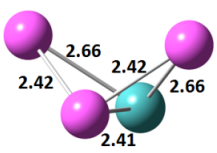
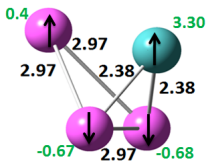
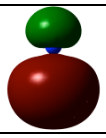
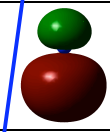
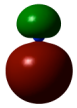
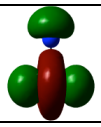
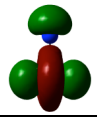
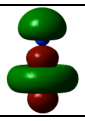
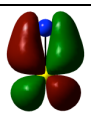
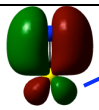
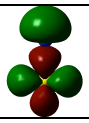
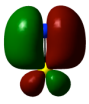
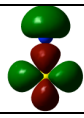
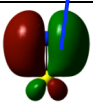
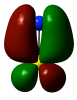
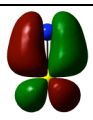
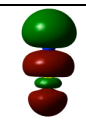
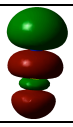
Ground state	**Cationic ground state**	**Nearest spin states of the ground state isomer**	**Next low energy isomers**	
				
μ_{tot}=4, ΔE=0	**μ_{tot}=5, ΔE=7.07eV**	**μ_{tot}=2, ΔE=0.26eV**		
				
		μ_{tot}=6, ΔE=0.57eV		
				
μ_{tot}=2, ΔE=0	**μ_{tot}=3, ΔE=7.26eV**	**μ_{tot}=4, ΔE=0.56eV**	**μ_{tot}=0, ΔE=0.54eV**	**μ_{tot}=0, ΔE=0.53eV**
				
μ_{tot}=0, ΔE=0	**μ_{tot}=1, ΔE=7.62eV**	**μ_{tot}=2, ΔE=1.31eV**	**μ_{tot}=0, ΔE=0.002eV**	**μ_{tot}=2, ΔE=1.36eV**

Fig. 1Sd. Electronic configurations and different valance electron orbitals of small sized Ge-Mo clusters in different spin states. The blue arrows represent the change of electronic state when the cluster shifted from lower to higher spin state.

GeMo Triplet			GeMo Quintet		GeMo Septet	
α orbital	ß orbital		α orbital	ß orbital	α orbital	ß orbital
						
					π:4.29	
						
			π:5.19		π:5.52	
						
π:5.27			π:6.06		π:6.36	
						
σ:6.28			σ:6.09		σ:6.39	
						
π:6.44	π:5.25		π:6.14		π:6.58	
						
π:6.44	π:5.25		π:6.25	π:4.97	π:6.74	
						
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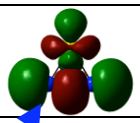
σ:11.21	σ:12.13		σ:11.70	σ:12.19	σ:12.65	σ:11.64

Ge-Mo: Triplet: $\sigma s^2\, \sigma s^2\, \pi p^2\, \pi p^2\, \sigma s^1\, \pi p^1$

Quintet: $\sigma s^2\, \sigma s^2\, \pi p^2\, \pi p^1\, \sigma s^1\, \pi p^1\, \pi p^1$

Septet: $\sigma s^2\, \sigma s^2\, \pi p^1\, \pi p^1\, \sigma s^1\, \pi p^1\, \pi p^1\, \pi p^1$

Fig. 1d contd.

Ge(2)Mo Triplet		Ge(2)Mo Quintet		Ge(3)Mo Singlet		Ge(3)Mo Triplet	
α orbital	ß orbital	α orbital	ß orbital	α orbital	ß orbital	α orbital	ß orbital
							
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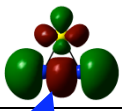
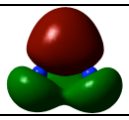
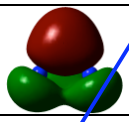
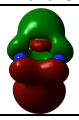
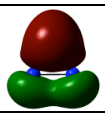
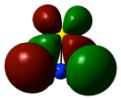
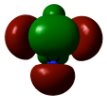
							
		B1:4.70		A′:5.74	A′:5.74	A′:6.14	
							
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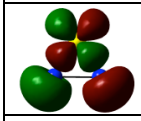		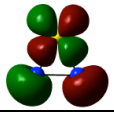		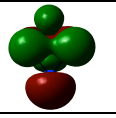	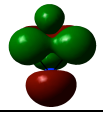	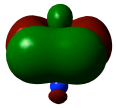	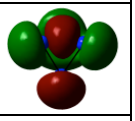
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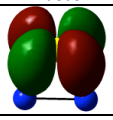	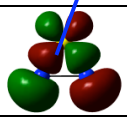	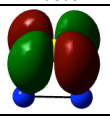		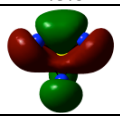	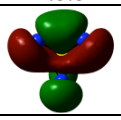	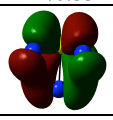	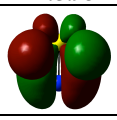
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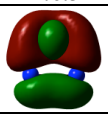
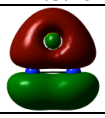
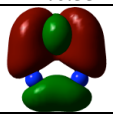
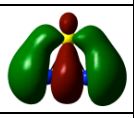
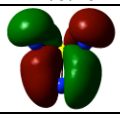
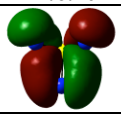
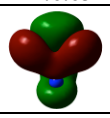
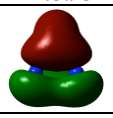
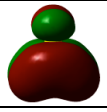
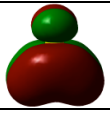
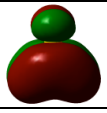
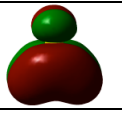
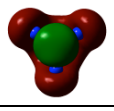
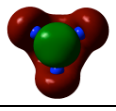
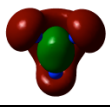
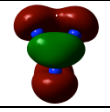
							
`A1:6.39	A1:5.79	A1:6.58	A1:5.44	A″:6.23	A″:6.23	A″:6.82	A″:6.14
							
B1:6.58	B1:5.93	B1:7.07	B1:5.74	A′:6.80	A′:6.80	A′:7.34	A′:6.69
A1:6.61	A1:6.25	A1:7.07	A1:5.93	A′:11.59	A′:11.59	A′:11.29	A′:11.04
B2:10.82	B2:11.21	B2:10.44	B2:10.26	A″:11.59	A″:11.59	A″:11.86	A″:12.10
A1:13.57	A1:13.93	A1:13.98	A1:15.75	A′:13.95	A′:13.95	A′:14.66	A′:14.66

Ge(2)Mo: Triplet: $(3a_1)^2\ 2(b_2)^2\ 4(a_1)^2\ 2(b_1)^2\ 5(a_1)^2\ 1(a_2)^2\ 3(b_2)^1\ 6(a_1)^1$;

Quintet: $(3a_1)^2\ 2(b_2)^2\ 4(a_1)^2\ 2(b_1)^2\ 5(a_1)^2\ 1(a_2)^1\ 3(b_2)^1\ 6(a_1)^1\ 3(b_1)^1$

Ge(3)Mo: Singlet: $1(A')^2\ 1(A'')^2\ 2(A')^2\ 3(A')^2\ 2(A'')^2\ 4(A')^2\ 5(A')^2 3(A'')^2 6(A')^2$

Triplet: $1(A')^2\ 1(A'')^2\ 2(A')^2\ 3(A')^2\ 2(A'')^2\ 4(A')^2\ 5(A')^2 3(A'')^2 6(A')^1\ 7(A')^1$

Fig. 2S. Variation of Mulliken charge on Mo atom with the cluster size (n).

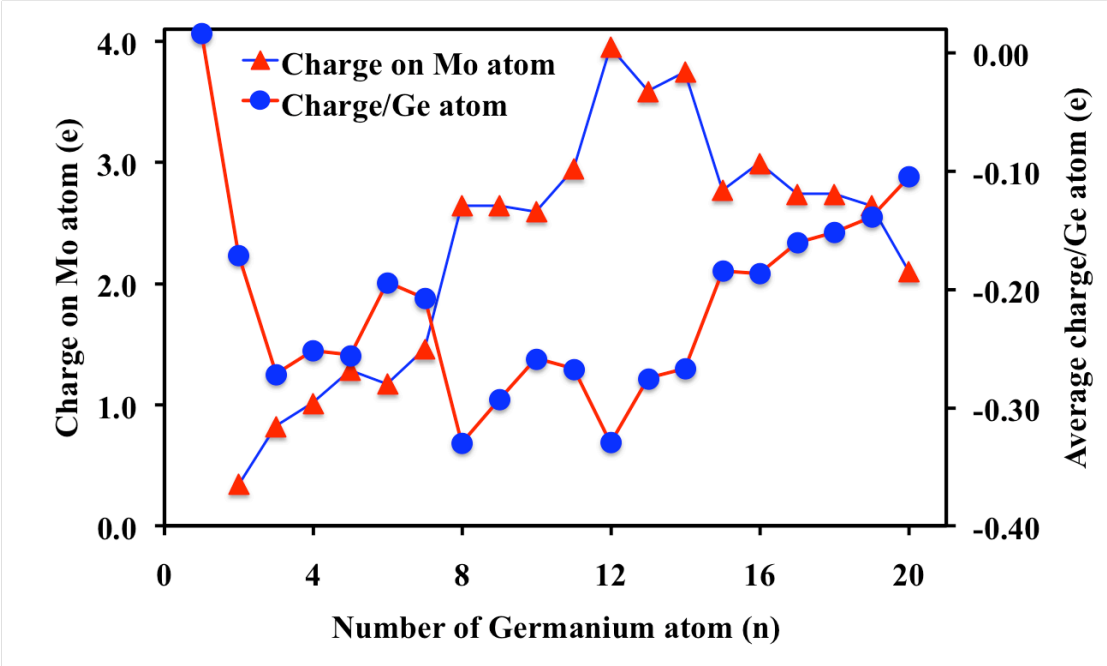


Fig. 3S. Site projected density of states plot of different Mo@Ge_n clusters with the contribution of Mo d-orbital (in red).

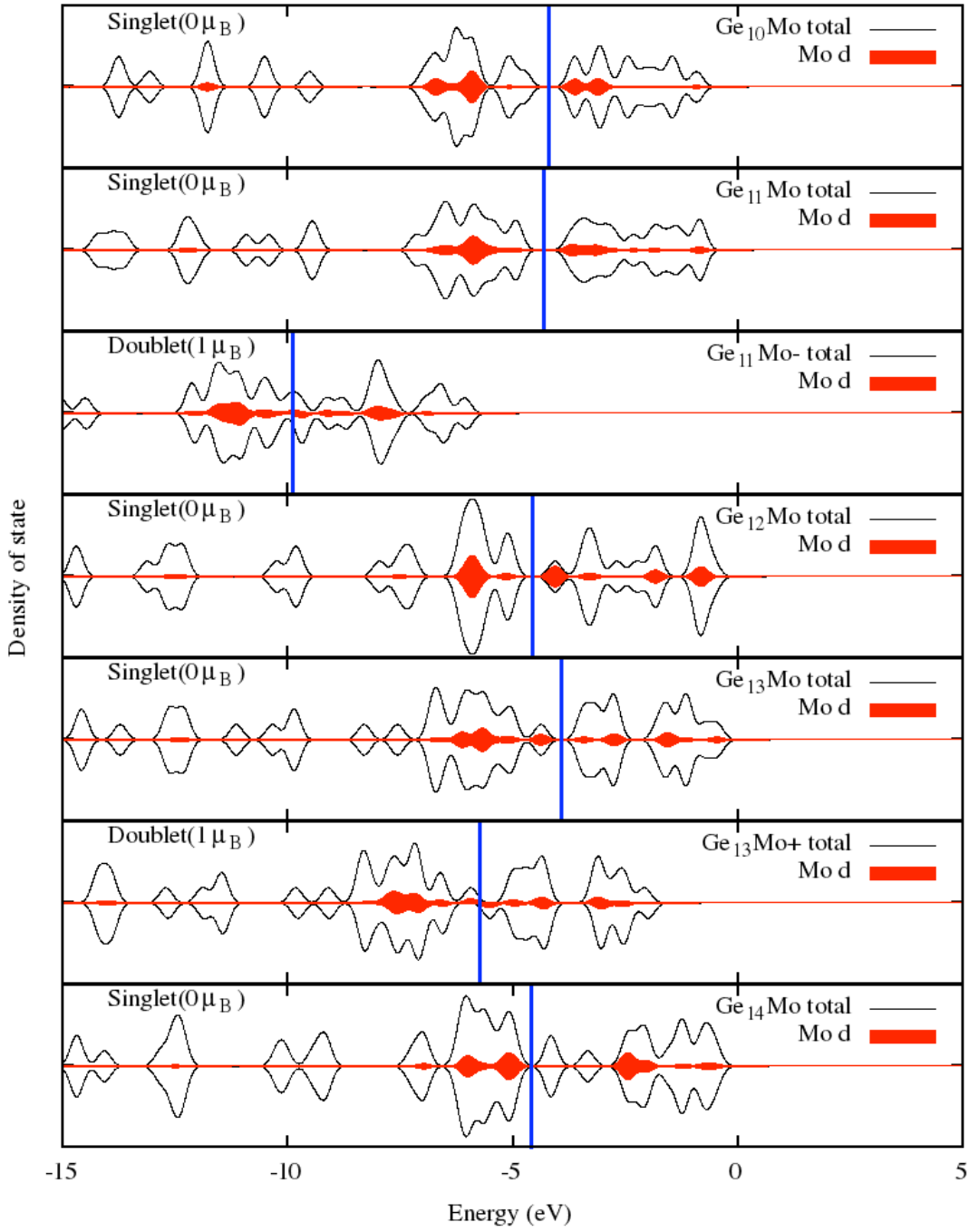


Fig. 4S. Variation of HOMO-LUMO gap of neutral and cationic of $Mo@Ge_n$ clusters with the cluster size (n)

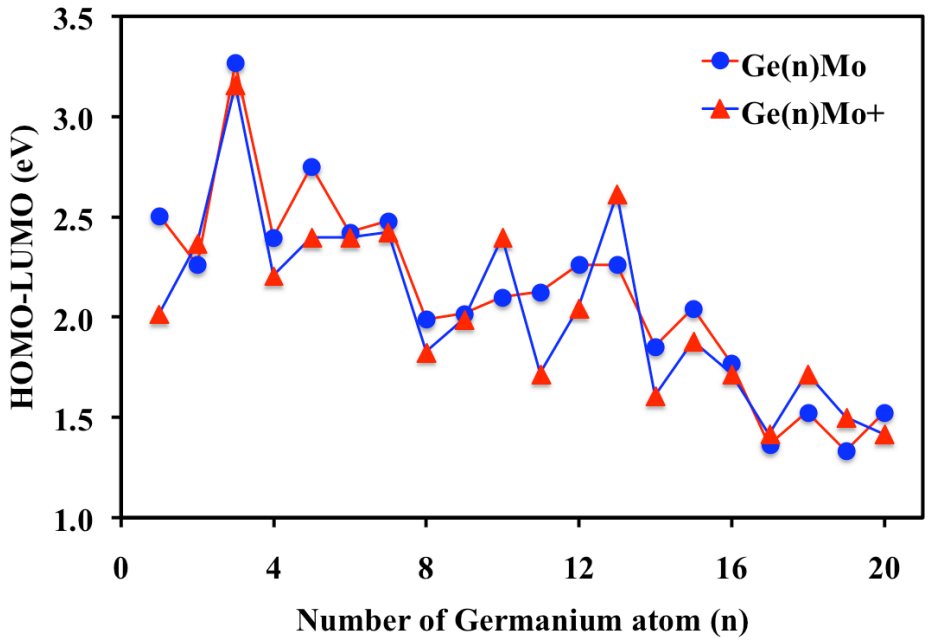
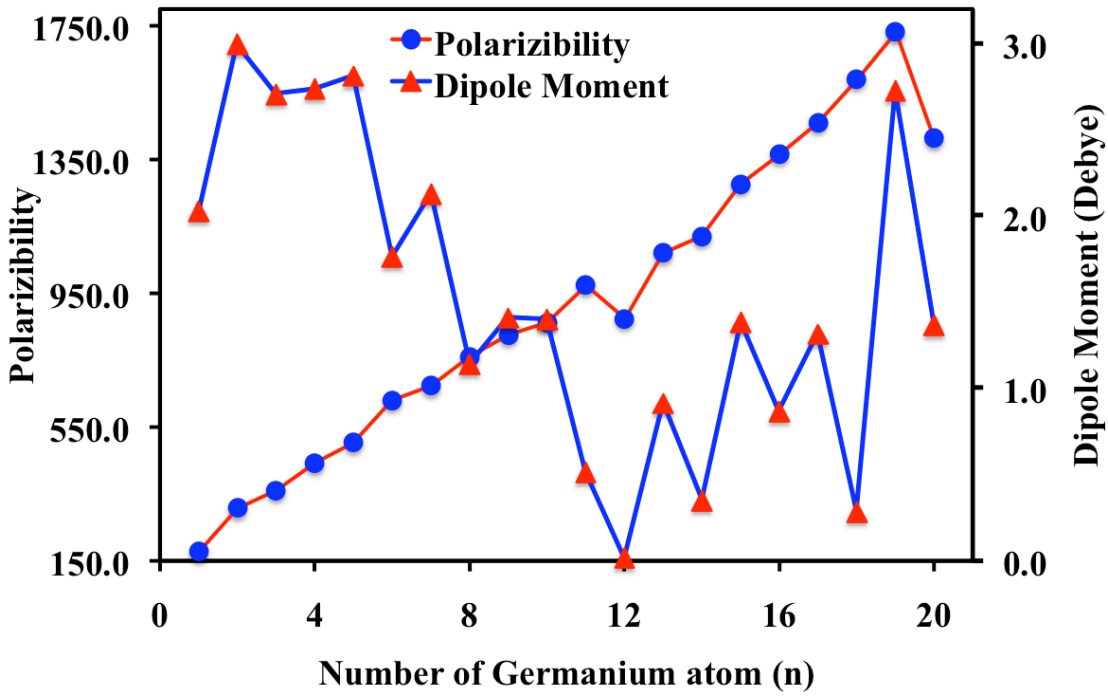


Fig. 5S. Variation of exact polarizability and dipole moment of $Mo@Ge_n$ clusters with the cluster size (n)



List of ESI figures

Fig. 1Sa. Optimized structures of Ge_n Mo (n=1-20) clusters with point group symmetry and relative energy (Kcal/mol) with respect to the ground state isomer in each size. Blue balls are Ge and yellow balls are Mo atoms.

Fig.1Sb. Different valence orbital's of $Mo@Ge_{12}$ in neutral and different charged state

Fig. 1Sc. Onsite magnetic moment of low energy neutral and cationic isomers with the bond lengths and relative energies with respect to the ground state neutral cluster. Dip blue balls are Mo and pink balls are Ge. Onsite magnetc moment is written in green in terms of μ_B.

Fig. 1Sd. Electronic configurations and different valance electron orbitals of small sized Ge-Mo clusters in different spin states. The blue arrows represent the change of electronic state when the cluster shifted from lower to higher spin state.

Fig. 2S. Variation of Mulliken charge on Mo atom with the cluster size (n).

Fig. 3S. Site projected density of states plot of different $Mo@Ge_n$ clusters with the contribution of Mo d-orbital (in red).

Fig. 4S. Variation of HOMO-LUMO gap of neutral and cationic of $Mo@Ge_n$ clusters with the cluster size (n)

Fig. 5S. Variation of exact polarizability and dipole moment of $Mo@Ge_n$ clusters with the cluster size (n)

Additional information not mentioned in the paper

Results of the calculations using M06 functional. VIP and VDE are not described in the manuscript.

Cluster	VIP (eV)	VDE (eV)	△ (eV)	HOMO-LUMO (eV)
Ge_8Mo	7.05	2.41	2.48	1.98
Ge_9Mo	7.21	2.8	3.13	2.01
$Ge_{10}Mo$	7.12	2.37	3.25	2.31
$Ge_{11}Mo$	7.3	2.99	2.68	2.09
$Ge_{12}Mo$	7.52	3.07	3.48	2.25
$Ge_{13}Mo$	6.82	2.49	2.65	2.25
$Ge_{14}Mo$	7.25	3.13	2.95	1.85
$Ge_{15}Mo$	7.02	3.2	2.8	2.04
$Ge_{16}Mo$	6.92	3.03	2.64	1.76
Ge_8	7.55	3.19	2.38	2.03
Ge_9	7.53	2.97	3.41	2.67
Ge_{10}	7.62	3.47	3.69	2.67
Ge_{11}	6.97	3.06	2.73	2.12
Ge_{12}	6.79	3.41	3.03	1.65
Ge_{13}	6.99	2.95	3.18	2.3
Ge_{14}	7.22	3.49	3.15	1.9
Ge_{15}	7.24	3.35	2.97	2.1
Ge_{16}	6.76	3.23	3.65	1.74

The shaded values represent the maximum stability of $Ge_{12}Mo$ cluster in M06 calculations. The values are comparable to the values obtained from the present calculations. As example, the IP calculated in the present calculation is 7.36 eV (Fig. 3), and the VIP obtained from M06 is 7.52 eV.

Optimization energies using M06 functional			
Cluster	**Neutral (eV)**	**Anion (eV)**	**Cation (eV)**
Ge_8Mo	-2674.835075	-2677.177302	-2667.94695
Ge_9Mo	-2778.691736	-2781.101523	-2771.551668
$Ge_{10}Mo$	-2882.474708	-2884.668394	-2875.065729
$Ge_{11}Mo$	-2985.939857	-2988.654107	-2978.65835
$Ge_{12}Mo$	-3089.197582	-3092.003526	-3081.812886
$Ge_{13}Mo$	-3193.475492	-3196.108442	-3187.046948

Calculated thermodynamic parameters (presented in the manuscript) using M06 functional

Clusters	B.E. (eV)	HOMO-LUMO gap (eV)	IP (eV)	Chemical potential (eV)	Chemical hardness (eV)
Ge_8Mo	2.4981	2.12	6.88	-4.61	2.272
Ge_9Mo	2.5627	2.28	7.14	-4.77	2.365
$Ge_{10}Mo$	2.6291	2.42	7.40	-4.80	2.607
$Ge_{11}Mo$	2.6305	2.20	7.28	-4.99	2.283
$Ge_{12}Mo$	2.6964	2.36	7.45	-5.09	2.289
$Ge_{12}Mo$	2.41	2.31	7.36	-5.21	2.15
$Ge_{13}Mo$	2.6937	1.57	6.42	-4.53	1.897

The shaded values, Pink and blue, represent the parameters of the most stable cluster $Ge_{12}Mo$ in the M06 calculations and in the present calculations respectively.

Details of Bonding-Anti-bonding, Occupancy and Energies of the states obtained from Gaussian output.

GeMo- Triplet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Mo(2)	1.0000	-0.25618	[**α**] Ge(1)-Mo(2)	0.00455	0.13929
[**β**] Ge(1)-Mo(2)	1.0000	-0.19411	[**β**] Ge(1)-Mo(2)	0.00027	-0.06821
Ge(1)-Mo(2)	1.0000	-0.19411	Ge(1)-Mo(2)	0.00027	-0.06821
Ge(1)-Mo(2)	1.0000	-0.26738	Ge(1)-Mo(2)	0.00337	0.10928
GeMo-Quintet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Mo(2)	1.0000	-0.26156	Ge(1)-Mo(2)	0.00361	0.11040
Ge(1)-Mo(2)	1.0000	-0.23654	Ge(1)-Mo(2)	0.00037	-0.08635
[**β**] Ge(1)-Mo(2)	1.0000	-0.18426	Ge(1)-Mo(2)	0.00013	-0.03359
Ge(1)-Mo(2)	1.0000	-0.26523	Ge(1)-Mo(2)	0.00275	-0.12463
GeMo-Septet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Mo(2)	1.0000	-0.27649	Ge(1)-Mo(2)	0.00309	0.05693
Ge(1)-Mo(2)	1.0000	-0.24872	Ge(1)-Mo(2)	0.00034	-0.09783
[**β**] Ge(1)-Mo(2)	1.0000	-0.26091	Ge(1)-Mo(2)	0.00287	0.08840
Ge_2Mo-Singlet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Mo(3)	0.97967	-0.21495	Ge(1)-Mo(3)	0.02066	-0.06281
Ge(1)-Mo(3)	0.96407	-0.26883	Ge(1)-Mo(3)	0.04025	0.13854
Ge(2)-Mo(3)	0.97967	-0.21496	Ge(1)-Mo(3)	0.02066	-0.06279
Ge(2)-Mo(3)	0.96406	-0.26885	Ge(2)-Mo(3)	0.04024	-0.13857
[**β**] Ge(1)-Mo(3)	0.97967	-0.21495	Ge(1)-Mo(3)	0.02066	-0.06281
Ge(1)-Mo(3)	0.96407	-0.26883	Ge(1)-Mo(3)	0.04025	0.13854
Ge(2)-Mo(3)	0.97967	-0.21496	Ge(1)-Mo(3)	0.02066	-0.06279
Ge(2)-Mo(3)	0.96406	-0.26885	Ge(2)-Mo(3)	0.04024	-0.13857
Ge_2Mo-Triplet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(2)-Mo(3)	0.85843	-0.21765	Ge(2)-Mo(3)	0.01555	-0.07941
Ge(2)-Mo(3)	0.83382	-0.20142	Ge(2)-Mo(3)	0.04853	-0.2518
Ge(2)-Mo(3)	0.78283	-0.22944	Ge(2)-Mo(3)	0.01428	-0.01278
[**β**] Ge(2)-Mo(3)	0.83083	-0.24044	Ge(2)-Mo(3)	0.01236	0.17348
Ge(2)-Mo(3)	0.67709	-0.17006	Ge(2)-Mo(3)	0.00050	-0.06609
Ge(2)-Mo(3)	0.65675	-0.14494	Ge(2)-Mo(3)	0.02371	-0.03275

Ge2Mo-Quintet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(2)-Ge(2)	0.96728	-0.19264	Ge(2)-Ge(2)	0.06799	-0.09631
Ge(1)-Mo(3)	0.94440	-0.26855	Ge(1)-Mo(3)	0.05834	0.05449
Ge(2)-Mo(3)	0.94441	-0.26855	Ge(2)-Mo(3)	0.05834	0.05448
[**β**] Ge(2)-Ge(2)	0.79132	-0.24481	Ge(2)-Ge(2)	0.00070	0.06262
Ge(1)-Mo(3)	0.97188	-0.26181	Ge(1)-Mo(3)	0.03174	0.8488
Ge(1)-Mo(3)	0.97188	-0.26181	Ge(1)-Mo(3)	0.03174	0.8488
Ge3Mo Singlet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Mo(4)	0.96170	-0.28717	Ge(1)-Mo(4)	0.12282	0.13830
Ge(1)-Mo(4)	0.80477	-0.19262	Ge(1)-Mo(4)	0.05436	-0.06888
Ge(3)-Mo(4)	0.96170	-0.28717	Ge(3)-Mo(4)	0.12283	0.13829
Ge(3)-Mo(4)	0.80476	-0.19267	Ge(3)-Mo(4)	0.05436	-0.06888
[**β**] Ge(1)-Mo(4)	0.96170	-0.28717	Ge(1)-Mo(4)	0.12282	0.13830
Ge(1)-Mo(4)	0.80477	-0.19262	Ge(1)-Mo(4)	0.05436	-0.06888
Ge(1)-Mo(4)	0.96170	-0.28717	Ge(3)-Mo(4)	0.12283	0.13829
Ge(1)-Mo(4)	0.80476	-0.19264	Ge(3)-Mo(4)	0.05436	-0.06888
Ge3Mo-Triplet					
Bonding	**Occupancy**	**Energy**	**Antibonding**	**Occupancy**	**Energy**
[**α**] Ge(1)-Ge(3)	0.94212	-0.27897	Ge(1)-Ge(3)	0.00679	0.11782
Ge(2)-Mo(4)	0.99153	-0.28858	Ge(2)-Mo(4)	0.14066	0.06488
Ge(2)-Mo(4)	0.91651	-0.22519	Ge(2)-Mo(4)	0.03422	-0.06884
Ge(3)-Mo(4)	0.96640	-0.28009	Ge(3)-Mo(4)	0.18024	0.00935
[**β**] Ge(1)-Ge(3)	0.74567	-0.22324	Ge(2)-Mo(4)	0.01705	0.05321
Ge(2)-Mo(4)	0.78437	-0.20229	Ge(2)-Mo(4)	0.21865	0.02794
Ge(2)-Mo(4)	0.76495	-0.17730	Ge(2)-Mo(4)	0.00691	-0.06379