Supporting Information for

Theoretical studies of electronic structures, magnetic properties and electron conductivities on one-dimensional Ni_n (n = 3, 5, 7) complexes.

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Table S1 Calculated total energies and $\langle S^2 \rangle$ values of **1-NCS – 3-Cl** for the J_{ab} values.

	AF state		FM state	
Complexes	Total energy / a.u.	$\langle S^2 \rangle$	Total energy / a.u.	$\langle S^2 \rangle$
1-NCS	-7706.105045	1.9834	-7706.103010	6.0135
2-Cl [a]	-11866.271335	2.2847	-11866.271105	6.2900
2-Cl [b]	-11866.271340	2.2783	-11866.271110	6.2842
2-CN	-11131.352064	2.0226	-11131.351887	6.0283
2-NNN	-11274.064323	2.2707	-11274.064182	6.2814
2-NCS	-11928.827496	2.0194	-11928.827321	6.0234
3-Cl [a]	-16089.850089	2.2636	-16089.849973	6.2551
3-Cl [b]	-16089.850489	2.3977	-16089.850469	6.3972

a) in Polyhedron 2005, 24, 2751. b) This study.

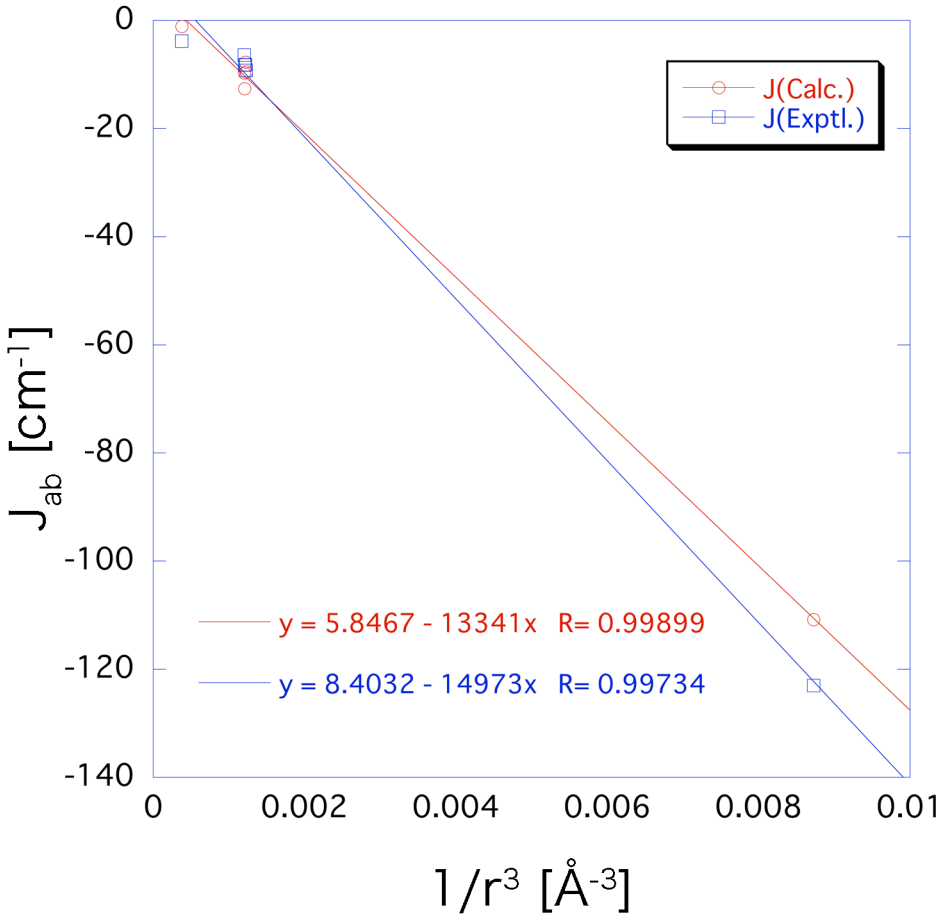
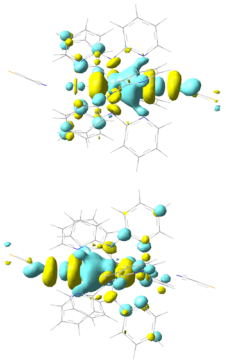
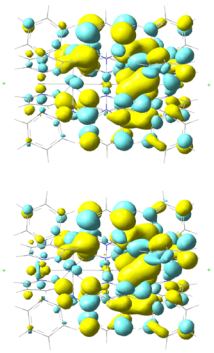
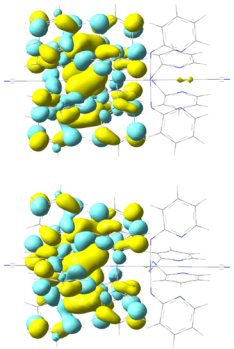
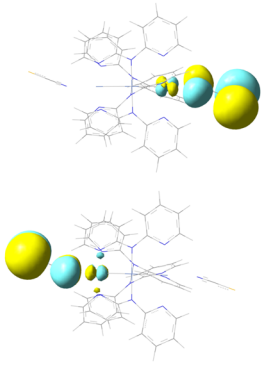
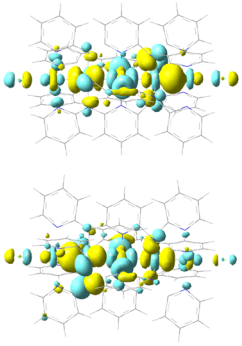
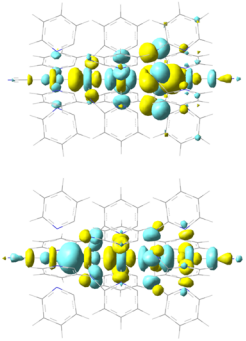


Fig S1 Least-square fits of J_{ab} by $1/r_{1\text{-}5}{}^{3}$

	1-NCS	**2-Cl**	**2-CN**
LUMO Upper : α Lower : β			
HOMO Upper : α Lower : β			

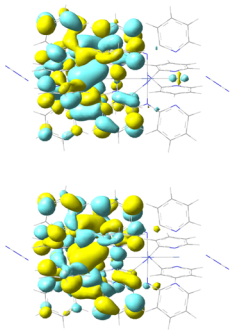
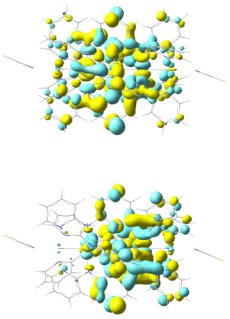
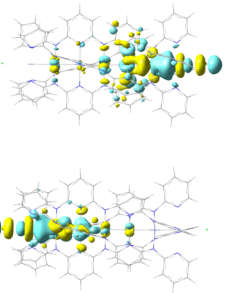
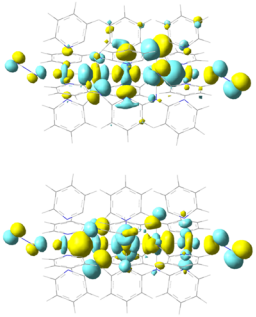
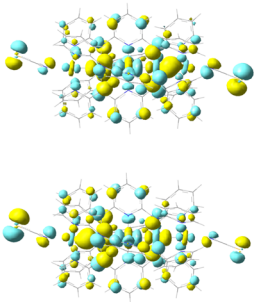
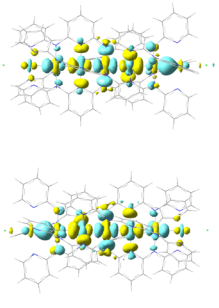
	2-N3	**2-NCS**	**3-Cl**
LUMO Upper : α Lower : β			
HOMO Upper : α Lower : β			

Fig S2 Depicted frontier orbitals of **1-NCS** – **3-Cl**.

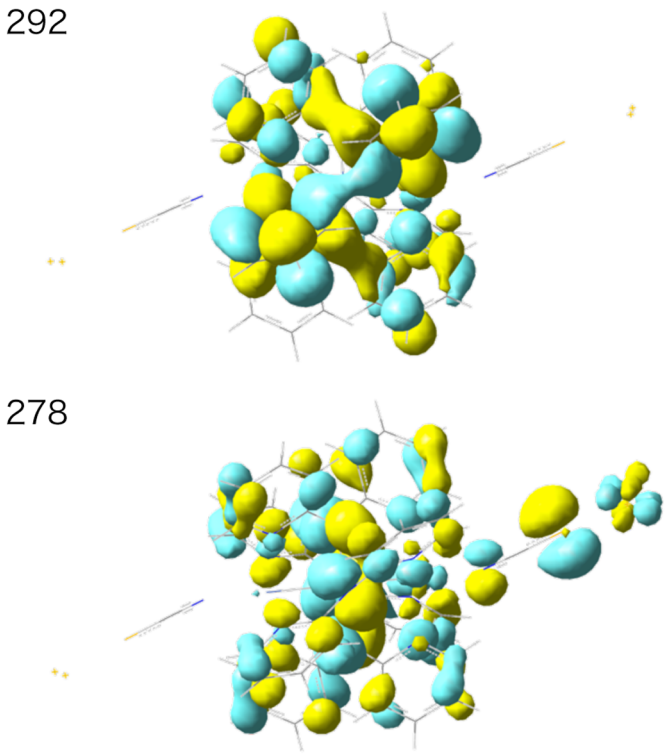


Fig S3 Additional MOs contributes to the conductivity.

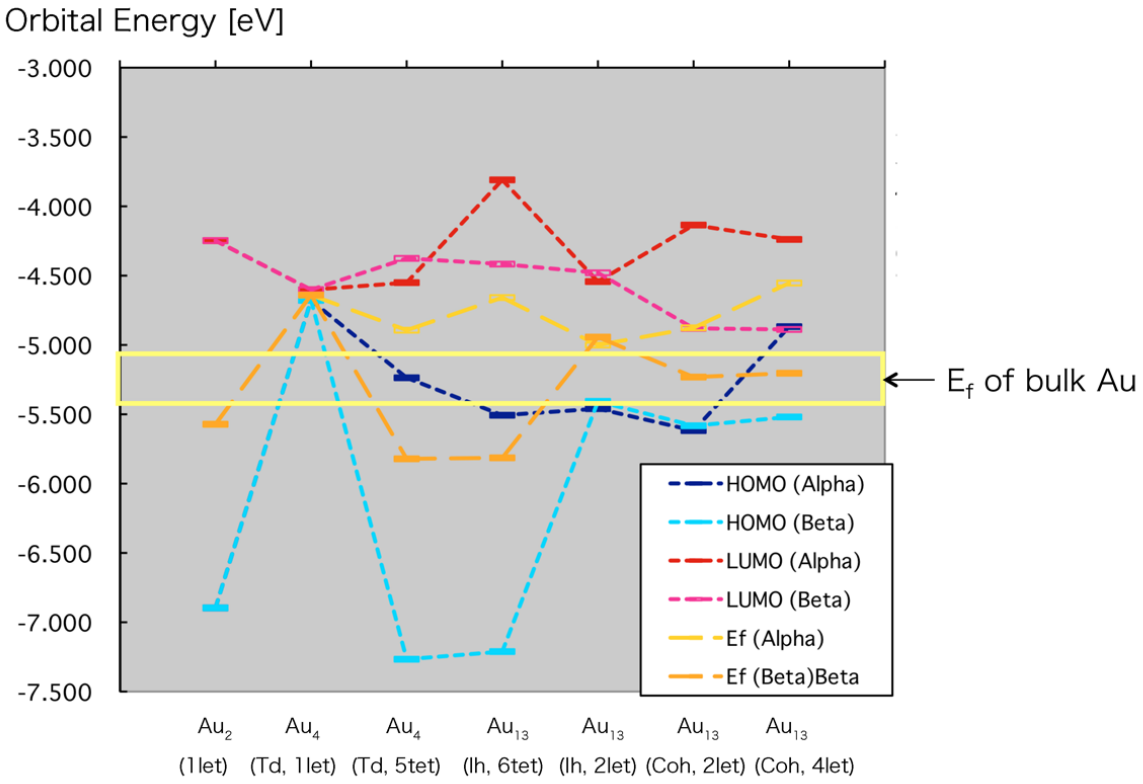


Fig S4 HOMO, LUMO and approximated E_F energies of Au clusters.
(Ih : Icosahedron, Coh : Cuboctahedron)

Table S2 Calculated $\left|\left\langle 1\left|\phi_{p,\sigma}\right\rangle\right|^2\left|\left\langle\phi_{p,\sigma}\left|N\right\rangle\right|^2\right.$ and γ values of **2-NCS**.

	γ				$\left\|\left\langle 1\left\|\phi_{p,\sigma}\right\rangle\right\|^2\left\|\left\langle\phi_{p,\sigma}\left\|N\right\rangle\right\|^2\right.$	
	α orbital		β orbital			
	site 1	site N	site 1	site N	α orbital	β orbital
<HOMO-9>	0.21886	0.00726	0.60998	0.62091	0.00000	0.14345
<HOMO-8>	0.85906	0.13045	0.22892	1.68246	0.01256	0.14834
<HOMO-7>	0.14429	0.78700	0.16227	0.23826	0.01289	0.00149
<HOMO-6>	0.06723	0.07732	0.02955	0.18806	0.00003	0.00003
<HOMO-5>	0.20289	0.07576	0.77852	0.04540	0.00024	0.00125
<HOMO-4>	1.50461	0.01259	0.20844	1.30205	0.00036	0.07365
<HOMO-3>	0.08105	0.19897	0.46013	0.09345	0.00026	0.00185
<HOMO-2>	0.01545	1.09280	1.66616	0.00821	0.00028	0.00019
<HOMO-1>	0.05266	1.07649	3.12120	0.23990	0.00321	0.56067
<HOMO-0>	0.30776	0.17665	0.48582	1.60993	0.00296	0.61172
<LUMO+0>	0.06213	0.00543	0.01843	0.55552	0.00000	0.00010
<LUMO+1>	0.00052	0.19702	0.74532	0.02650	0.00000	0.00039
<LUMO+2>	0.02180	0.18120	1.51558	0.07714	0.00002	0.01367
<LUMO+3>	0.00538	0.00397	1.86134	0.00661	0.00000	0.00015
<LUMO+4>	0.03143	0.02079	1.38463	0.01305	0.00000	0.00033
<LUMO+5>	0.01668	0.00145	0.22228	0.07029	0.00000	0.00024
<LUMO+6>	0.03546	0.05762	1.88783	0.19491	0.00000	0.13539
<LUMO+7>	0.01030	0.01678	0.91835	0.01098	0.00000	0.00010
<LUMO+8>	0.01028	0.00899	0.55073	0.00980	0.00000	0.00003
<LUMO+9>	0.02995	0.00299	0.67286	0.11074	0.00000	0.00555

Table S3 Calculated $\left|\left\langle 1\left|\phi_{p,\sigma}\right\rangle\right|^2\left|\left\langle\phi_{p,\sigma}\left|N\right\rangle\right|^2\right.$ and γ values of **1-NCS**.

	γ				$\left\|\left\langle 1\left\|\phi_{p,\sigma}\right\rangle\right\|^2\left\|\left\langle\phi_{p,\sigma}\left\|N\right\rangle\right\|^2\right.$	
	α orbital		β orbital			
	site 1	site N	site 1	site N	α orbital	β orbital
<HOMO-9>	1.43171	0.33161	0.62832	0.96545	0.22540	0.36797
<HOMO-8>	0.59055	0.31116	0.55050	0.22422	0.03377	0.01524
<HOMO-7>	0.00499	1.72177	1.80627	0.03311	0.00007	0.00358
<HOMO-6>	1.74677	0.01169	0.04695	1.70324	0.00042	0.00639
<HOMO-5>	0.02800	0.02033	0.04555	0.09243	0.00000	0.00002
<HOMO-4>	0.05648	0.03823	0.07491	0.04932	0.00000	0.00001
<HOMO-3>	0.09581	0.02720	0.03324	0.05976	0.00001	0.00000
<HOMO-2>	0.10132	0.04061	0.08700	0.05542	0.00002	0.00002
<HOMO-1>	0.01426	0.65374	0.00551	0.64334	0.00009	0.00001
<HOMO-0>	0.11276	0.09755	0.13697	0.04025	0.00012	0.00003
<LUMO+0>	0.00003	0.28251	0.00001	0.26548	0.00000	0.00000
<LUMO+1>	0.04208	0.00001	0.02451	0.00005	0.00000	0.00000
<LUMO+2>	0.00377	0.00151	0.00003	0.08823	0.00000	0.00000
<LUMO+3>	0.04092	0.00381	0.00804	0.01666	0.00000	0.00000
<LUMO+4>	0.00717	0.00027	0.00519	0.00046	0.00000	0.00000
<LUMO+5>	0.01116	0.00032	0.01068	0.00003	0.00000	0.00000
<LUMO+6>	0.00602	0.01771	0.01197	0.03169	0.00000	0.00000
<LUMO+7>	0.01033	0.00432	0.00518	0.00989	0.00000	0.00000
<LUMO+8>	0.00107	0.00831	0.00566	0.02262	0.00000	0.00000
<LUMO+9>	0.00279	0.02078	0.00904	0.01851	0.00000	0.00000