Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Conductive Metal Adatom Adsorbed on Graphene Nanoribbons: A First-Principles Study of Electronic Structures, Magnetization and Transport Properties

Cai Xia Wu,[a] Shi Zheng Wen,[b] Li Kai Yan*,[a] Min Zhang*,[a] Teng Ying Ma,[a] Yu He Kan,[b] Zhong Min Su*[a]

Table S1 Parameters for single adatom adsorbed on 7ZGNR. E_{ad} is the adsorption energy, Δq is the charge transfer from metal adatom to 7ZGNR, m_{cell} is the magnetic moment, h is the distance of the adatom above 7ZGNR, d_{M-C} is the distance between the metal adatom and the nearest carbon atoms, Δd is the maximum deviation in the z direction of the C atoms in 7ZGNR from the average positions.

		h (Å)	d_{M-C} (Å)	Δd (Å)	E_{ad} (eV)	Δq (e/atom)	m_{cell} (μ_B)
Al	H	2.249	2.016	0.487	-2.358	0.094	-1.005
Cu	T	2.651	2.138	0.636	-1.546	-0.004	-1.001
Ag	T	2.907	2.311	0.597	-0.975	0.090	-1.006
Au	T	2.958	2.377	0.584	-0.930	0.203	-1.012

Table S2 Parameters for two metal adatoms adsorbed on 6ZGNR. E_{ad} is the dimer adsorption energy which treats the two metal adatoms (M_2) as a single entity defined as $E_{ad} = E_{tot} - E_{M2} - E_g$, and the number in the parenthesis is the binding energy E_b defined as $E_b = E_{tot} - 2E_M - E_g$, where E_M stands for the energy of the single adatom. d_{M-M} is the distance between two metal adatoms.

		h (Å)	d_{M-C} (Å)	Δd (Å)	d_{M-M} (Å)	E_{ad} (E_b) (eV)	Δq (e/M_2)	m_{cell} (μ_B)
Al	H	2.165	2.273	0.196	4.903	-4.510 (-4.082)	0.180	-1.583
Cu	T	2.650	2.109	0.558	2.437	-1.073 (-3.096)	-0.216	-1.595
Ag	T	2.951	2.497	0.475	2.789	-0.392 (-1.949)	-0.056	-0.366
Au	T	3.500	3.428	0.122	2.806	-0.167 (-1.787)	-0.004	-0.018

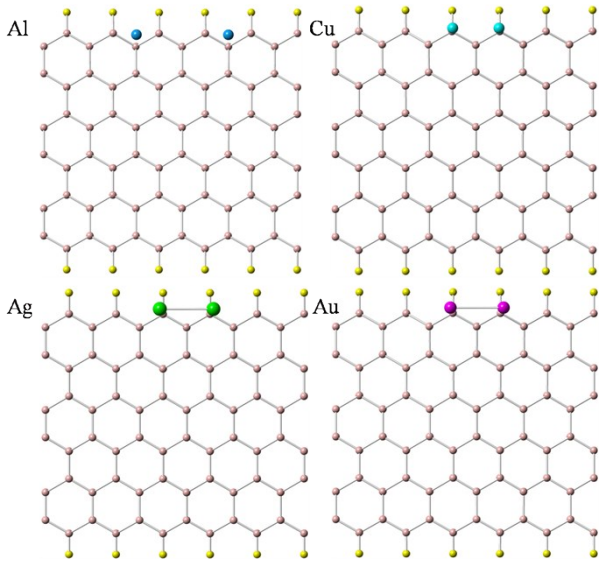

Fig. S1 The most stable structures for Al, Cu, Ag and Au on 6ZGNR.

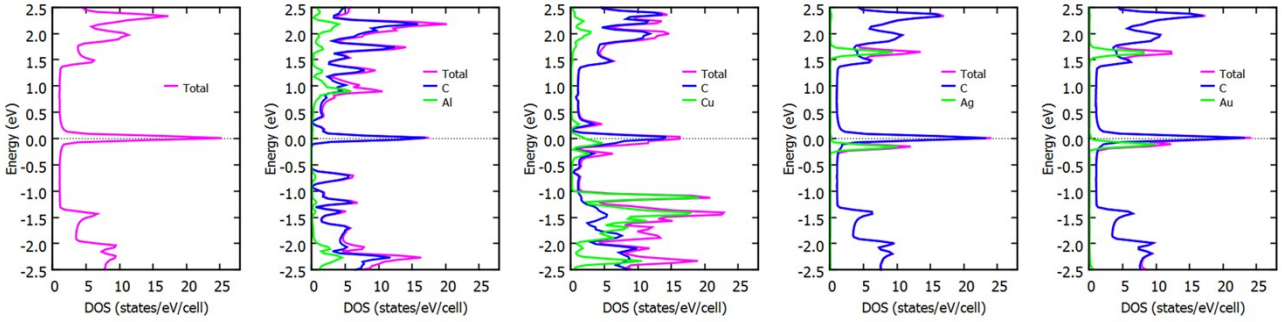

Fig. S2 PDOS for 6ZGNR-based scattering region.

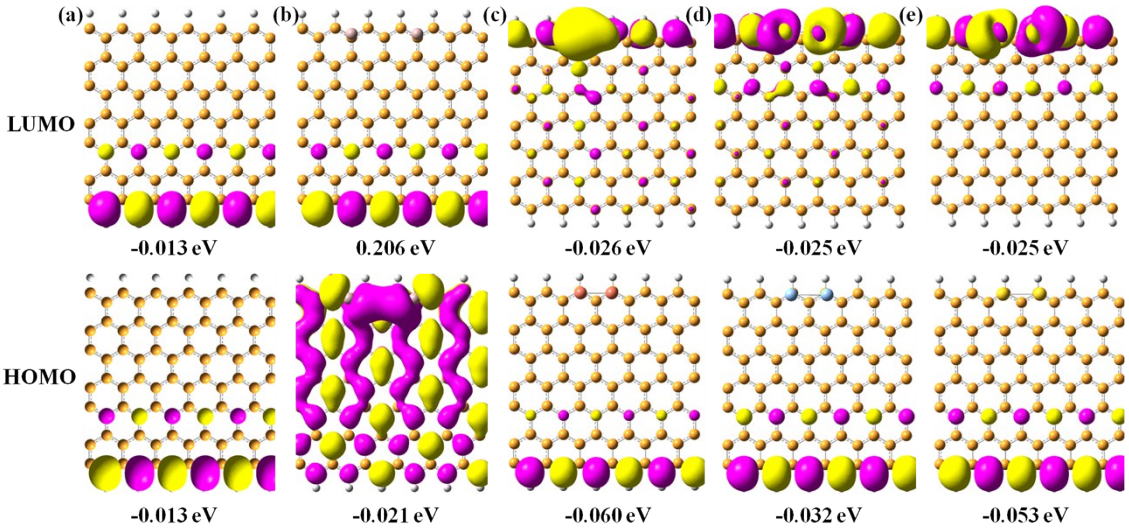

Fig. S3 Frontier molecular orbitals for pure 7ZNGR (a) and 7ZGNR with Al (b), Cu (c), Ag (d) and Au (e) atom.

Optimized structures of ZGNR with different metal atoms

ZGNR-Al:

	X	Y	Z
C	11.011678	0.587792	7.291708
C	8.840828	1.820625	7.225684
C	8.148608	0.588192	7.162406
C	10.293157	1.818544	7.286840
C	15.333388	0.587624	7.420902
C	13.172008	1.818290	7.385096
C	12.452002	0.587427	7.345426
C	14.612137	1.818060	7.419874
C	19.644272	0.588094	7.496825
C	17.493804	1.818220	7.466995
C	16.775659	0.587815	7.449131
C	18.947344	1.818504	7.487258
C	11.008416	3.045576	7.380278
C	8.833965	4.273568	7.438084
C	8.144646	3.053537	7.286266
C	10.285966	4.272744	7.463413
C	15.331622	3.047889	7.464897
C	13.168531	4.276895	7.502672
C	12.449819	3.047233	7.418412
C	14.608970	4.277417	7.510256
C	19.643345	3.049253	7.495978
C	17.491305	4.278631	7.504767
C	16.774335	3.047844	7.477570
C	18.945318	4.278885	7.498918
C	11.002828	5.498353	7.582689
C	8.823541	6.714071	7.733251
C	8.135616	5.506442	7.590191
C	10.278781	6.723127	7.697857
C	15.327624	5.507918	7.559148
C	13.163371	6.735814	7.642999
C	12.445948	5.504380	7.581097
C	14.604873	6.736943	7.612811
C	19.641072	5.509542	7.496389
C	17.489061	6.738090	7.550368
C	16.770906	5.508019	7.539621
C	18.943052	6.738546	7.515931
C	10.997237	7.966765	7.739091
C	8.822306	9.219504	7.728112
C	8.152948	7.967309	8.060561

C	10.278610	9.211316	7.698397
C	15.326274	7.967640	7.613137
C	13.162945	9.199066	7.643080
C	12.440887	7.967337	7.691926
C	14.604594	9.198361	7.612516
C	19.639721	7.968198	7.498217
C	17.488962	9.197790	7.549855
C	16.769174	7.967872	7.575821
C	18.942989	9.197810	7.515560
C	11.002384	10.437344	7.584514
C	8.833437	11.663392	7.444246
C	8.134876	10.431232	7.598598
C	10.285744	11.662794	7.465820
C	15.327415	10.427394	7.558465
C	13.168266	11.658085	7.502821
C	12.445516	10.430888	7.581976
C	14.608690	11.657757	7.509622
C	19.640994	10.426833	7.495936
C	17.491164	11.657122	7.503667
C	16.770710	10.427714	7.538725
C	18.945204	11.657364	7.498132
C	11.008274	12.889960	7.381360
C	8.840553	14.115721	7.227381
C	8.143999	12.883109	7.290785
C	10.293011	14.116983	7.287818
C	15.331490	12.887316	7.464046
C	13.171865	14.116788	7.384913
C	12.449646	12.887704	7.418553
C	14.612027	14.117008	7.419465
C	19.643356	12.886960	7.495470
C	17.493820	14.117507	7.466388
C	16.774200	12.887870	7.476523
C	18.947336	14.117645	7.486830
H	7.041975	0.588527	7.113929
H	20.751701	0.588209	7.516020
H	7.037816	3.052881	7.254812
H	20.750525	3.051195	7.505336
H	7.028247	5.503139	7.591810
H	20.748001	5.511445	7.478726
H	7.044161	7.968227	8.034470
H	20.746075	7.968268	7.463470
H	7.027386	10.435055	7.598587
H	20.747917	10.425056	7.478827
H	7.037049	12.884414	7.259820

H	20.750442	12.885334	7.505404
Al	9.028026	8.070313	10.068440

ZGNR-Cu:

	X	Y	Z
C	11.007617	0.610969	7.264574
C	8.835837	1.845619	7.212193
C	8.143214	0.610790	7.147194
C	10.289188	1.843695	7.268457
C	15.331035	0.611051	7.392468
C	13.169047	1.842479	7.356290
C	12.448747	0.611050	7.314420
C	14.609898	1.841921	7.391118
C	19.642860	0.610646	7.494492
C	17.491795	1.841215	7.452705
C	16.773185	0.610925	7.428902
C	18.945825	1.840670	7.481933
C	11.005997	3.071565	7.370836
C	8.836766	4.302359	7.445738
C	8.143909	3.083992	7.280164
C	10.287119	4.300295	7.475034
C	15.329898	3.071559	7.444384
C	13.167213	4.301448	7.492141
C	12.447934	3.071895	7.401272
C	14.607880	4.301366	7.495629
C	19.642453	3.070771	7.496457
C	17.490942	4.301249	7.497401
C	16.772773	3.071155	7.462782
C	18.944913	4.300953	7.497595
C	11.002749	5.527621	7.609494
C	8.834471	6.733668	7.839008
C	8.145090	5.538440	7.630266
C	10.284057	6.751285	7.759985
C	15.328177	5.531139	7.548590
C	13.165478	6.759775	7.646921
C	12.446228	5.529709	7.587055
C	14.606868	6.760775	7.605821
C	19.642031	5.530894	7.500172
C	17.490439	6.760489	7.545631
C	16.771417	5.530989	7.531826
C	18.944632	6.760536	7.517082
C	11.001909	7.991090	7.779525

C	8.834188	9.248333	7.833418
C	8.127596	7.991591	8.152179
C	10.283949	9.230755	7.755800
C	15.329345	7.991030	7.604447
C	13.165495	9.222394	7.644324
C	12.441613	7.991152	7.703847
C	14.606919	9.221473	7.603806
C	19.641790	7.990528	7.503913
C	17.490486	9.221182	7.544667
C	16.771379	7.990975	7.568898
C	18.944673	9.220644	7.516681
C	11.002724	10.454155	7.602794
C	8.836874	11.678628	7.433823
C	8.144975	10.442670	7.618962
C	10.287113	11.681185	7.465867
C	15.328239	10.450907	7.545541
C	13.167247	11.680571	7.486647
C	12.446246	10.452393	7.581828
C	14.607914	11.680702	7.491488
C	19.642127	10.450196	7.499968
C	17.491059	11.680477	7.495543
C	16.771518	10.450895	7.529738
C	18.945019	11.680230	7.496842
C	11.006051	12.910057	7.363589
C	8.835923	14.135865	7.205931
C	8.144113	12.896973	7.268085
C	10.289226	14.138052	7.263581
C	15.329936	12.910527	7.441327
C	13.169109	14.139661	7.353422
C	12.447984	12.910032	7.395711
C	14.609936	14.140134	7.389046
C	19.642573	12.910382	7.496257
C	17.491861	14.140599	7.451828
C	16.772855	12.910640	7.460773
C	18.945929	14.140579	7.481582
H	7.036376	0.610832	7.104332
H	20.749382	0.610594	7.521754
H	7.036899	3.088864	7.244612
H	20.749839	3.070413	7.510332
H	7.037148	5.532169	7.657235
H	20.749231	5.530856	7.485616
H	7.043101	7.990725	7.903241
H	20.748727	7.990311	7.472768
H	7.036979	10.448558	7.643816

H	20.749313	10.449787	7.486300
H	7.037201	12.891875	7.230315
H	20.749913	12.910530	7.510876
Cu	8.113242	7.995420	10.168219

ZGNR-Ni:

	X	Y	Z
C	11.016389	0.619360	7.467372
C	8.844925	1.842741	7.513150
C	8.148410	0.619941	7.475667
C	10.296072	1.846792	7.500612
C	15.338584	0.620954	7.471983
C	13.176104	1.851191	7.476598
C	12.457240	0.620485	7.464472
C	14.616820	1.851000	7.474944
C	19.650149	0.621306	7.504713
C	17.498731	1.851516	7.487997
C	16.780693	0.621057	7.480668
C	18.952964	1.851384	7.499901
C	11.010577	3.077721	7.523720
C	8.833347	4.290376	7.628071
C	8.146951	3.073916	7.580989
C	10.285832	4.303479	7.569234
C	15.336330	3.081099	7.479697
C	13.173161	4.309550	7.503213
C	12.453209	3.080004	7.498806
C	14.613619	4.310495	7.487077
C	19.648895	3.081963	7.504390
C	17.496987	4.311234	7.480806
C	16.779004	3.081175	7.482085
C	18.951014	4.311441	7.493006
C	11.007833	5.535858	7.541780
C	8.840536	6.771448	7.552452
C	8.105651	5.533274	7.699099
C	10.294402	6.771224	7.541238
C	15.333721	5.540951	7.483191
C	13.169725	6.771054	7.506827
C	12.449244	5.538944	7.517900
C	14.611112	6.770868	7.490417
C	19.647629	5.541375	7.499921
C	17.496095	6.771000	7.476549
C	16.776948	5.541024	7.476477

C	18.950553	6.771126	7.488949
C	11.007835	8.006509	7.540625
C	8.833184	9.252649	7.625677
C	8.105494	8.009727	7.697327
C	10.285687	9.238860	7.567182
C	15.333796	8.000771	7.483087
C	13.173069	9.232374	7.502282
C	12.449111	8.002930	7.517133
C	14.613671	9.231151	7.486651
C	19.647723	8.000935	7.499853
C	17.496906	9.230543	7.480608
C	16.776834	8.000737	7.476403
C	18.951163	9.230742	7.492886
C	11.010511	10.464618	7.521853
C	8.844966	11.700321	7.511160
C	8.146798	10.469200	7.578308
C	10.296013	11.695731	7.499028
C	15.336289	10.460626	7.479185
C	13.176123	11.690762	7.475849
C	12.453158	10.462051	7.497526
C	14.616766	11.690925	7.474349
C	19.648974	10.460396	7.504389
C	17.498814	11.690209	7.487823
C	16.779101	10.460606	7.481756
C	18.952956	11.690801	7.499962
C	11.016400	12.923079	7.466760
C	8.844976	14.151567	7.460402
C	8.148434	12.923268	7.474578
C	10.297811	14.151346	7.458883
C	15.338477	12.920766	7.471609
C	13.178121	14.150973	7.459675
C	12.457210	12.921697	7.464107
C	14.618441	14.151029	7.466365
C	19.650098	12.920932	7.504766
C	17.499283	14.150894	7.484890
C	16.780738	12.920818	7.480429
C	18.953197	14.151155	7.497002
H	7.041250	0.621255	7.479992
H	20.757597	0.621886	7.513897
H	7.039818	3.070410	7.604179
H	20.755966	3.082737	7.514724
H	7.032662	5.511286	7.412721
H	20.754741	5.541980	7.519723
H	7.032890	8.031163	7.409347

H	20.754715	8.000422	7.519728
H	7.039728	10.472984	7.601369
H	20.756018	10.459739	7.514660
H	7.041236	12.922255	7.479146
H	20.757642	12.920785	7.513830
Ni	8.100464	6.772672	9.347416