Supporting Information

(non-) Periodic Variation of Excited-State Properties for Coinage Metal Dimers M_2 (M = Cu, Ag, Au, Rg)

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Table S1. Ionization potentials (eV) and electron affinity energies (eV) of the Cu_2 molecule.

SR		SOC	
IP		IP	
$^2\Sigma_g^+$	7.735	$(1/2)_g$ ($^2\Sigma_g^+$)	7.735
$^2\Sigma_u^+$	8.985	$(1/2)_u$ ($^2\Sigma_u^+$)	8.976
$^2\Pi_g$	9.125	$(3/2)_g$ ($^2\Pi_g$)	9.062
		$(1/2)_g$ ($^2\Pi_g$)	9.168
EA		EA	
$^2\Sigma_u^+$	-0.557	$(1/2)_u$ ($^2\Sigma_u^+$)	-0.557
$^2\Pi_u$	0.441	$(1/2)_u$ ($^2\Pi_u$)	0.438
$^2\Sigma_g^+$	0.503	$(3/2)_u$ ($^2\Pi_u$)	0.444
		$(1/2)_g$ ($^2\Sigma_g^+$)	0.503

Table S2. Ionization potentials (eV) and electron affinity energies (eV) of the Ag_2 molecule.

SR		SOC	
IP		IP	
$^2\Sigma_g^+$	7.616	$(1/2)_g$ ($^2\Sigma_g^+$)	7.607
$^2\Sigma_u^+$	11.052	$(1/2)_u$ ($^2\Sigma_u^+$)	11.027
$^2\Pi_g$	11.322	$(3/2)_g$ ($^2\Pi_g$)	11.183
		$(1/2)_g$ ($^2\Pi_g$)	11.404
EA		EA	
$^2\Sigma_u^+$	-0.876	$(1/2)_u$ ($^2\Sigma_u^+$)	-0.872
$^2\Pi_u$	0.331	$(1/2)_u$ ($^2\Pi_u$)	0.321
$^2\Sigma_g^+$	0.401	$(3/2)_u$ ($^2\Pi_u$)	0.340
		$(1/2)_g$ ($^2\Sigma_g^+$)	0.401

Table S3. Ionization potentials (eV) and electron affinity energies (eV) of the Au_2 molecule.

SR		SOC	
IP		IP	
$^2\Sigma_g^+$	9.301	$(1/2)_g$ ($^2\Sigma_g^+$)	9.287
$^2\Sigma_u^+$	10.073	$(3/2)_u$ ($^2\Pi_u$)	9.786
$^2\Pi_g$	10.262	$(1/2)_g$ ($^2\Sigma_g^+$)	9.927
		$(1/2)_g$ ($^2\Pi_g$)	10.475
EA		EA	
$^2\Sigma_u^+$	-1.661	$(1/2)_u$ ($^2\Sigma_u^+$)	-1.688
$^2\Pi_u$	0.336	$(1/2)_u$ ($^2\Pi_u$)	0.286
$^2\Sigma_g^+$	0.411	$(3/2)_u$ ($^2\Pi_u$)	0.369
		$(1/2)_g$ ($^2\Sigma_g^+$)	0.404

Table S4. Ionization potentials (eV) and electron affinity energies (eV) of the Rg_2 molecule.

SR		SOC	
IP		IP	
$^2\Pi_g$	9.973	$(3/2)_g$ ($^2\Pi_g$)	9.184
$^2\Delta_u$	10.240	$(5/2)_u$ ($^2\Delta_u$)	9.389
$^2\Delta_g$	10.770	$(5/2)_g$ ($^2\Delta_g$)	9.992
$^2\Sigma_u^+$	10.813	$(1/2)_g$ ($^2\Pi_g$)	10.101
$^2\Sigma_g^+$	11.653	$(3/2)_u$ ($^2\Delta_u$)	10.814
		$(1/2)_u$ ($^2\Sigma_u^+$)	10.853
		$(1/2)_g$ ($^2\Sigma_g^+$)	12.483
		$(3/2)_g$ ($^2\Delta_g$)	12.487
EA		EA	
$^2\Sigma_u^+$	-2.761	$(1/2)_u$ ($^2\Sigma_u^+$)	-2.827
$^2\Pi_u$	0.574	$(1/2)_u$ ($^2\Pi_u$)	0.228
$^2\Sigma_g^+$	1.478	$(1/2)_g$ ($^2\Sigma_g^+$)	0.664
		$(3/2)_u$ ($^2\Pi_u$)	1.175

Table S5. Bond length (Å), harmony frequency (cm^{-1}), adiabatic excitation energy (eV), and vertical excitation energies (eV) of Cu_2 based on EOM-CCSD.

		TZ				QZ				5Z			
State		R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e
SR													
$^1\Sigma_g^+$	$(1\sigma_g^+)^2$	2.242	0	0	255	2.237	0	0	255	2.235	0	0	256
$^3\Sigma_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	-	-	2.044	-	-	-	2.057	-	-	-	2.063	-
$^3\Sigma_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.229	2.257	2.255	251	2.223	2.333	2.331	251	2.222	2.367	2.366	252
$^3\Pi_u$	$\pi_g^1(2\sigma_u^+)^1$	2.234	2.351	2.349	248	2.229	2.428	2.427	248	2.227	2.464	2.463	250
$^1\Sigma_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.230	2.515	2.513	250	2.224	2.588	2.586	250	2.222	2.621	2.620	250
$^1\Pi_u$	$\pi_g^1(2\sigma_u^+)^1$	2.241	2.623	2.623	245	2.235	2.698	2.698	245	2.233	2.733	2.733	244
$^1\Sigma_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	2.380	2.704	2.794	215	2.376	2.741	2.826	214	2.373	2.759	2.841	215
SOC													
$0_g^+(1)$	$(^1\Sigma_g^+)$	2.242	0	0	255	2.237	0	0	255	2.235	0	0	256
$0_u^+(1)$	$(^3\Sigma_u^+)$	-	-	2.040	-	-	-	2.054	-	-	-	2.060	-
$1_u(1)$	$(^3\Sigma_u^+)$	-	-	2.041	-	-	-	2.054	-	-	-	2.061	-
0_g^-	$(^3\Sigma_g^+)$	2.233	2.246	2.244	249	2.226	2.321	2.320	249	2.225	2.356	2.355	251
1_g	$(^3\Sigma_g^+)$	2.232	2.247	2.245	250	2.226	2.322	2.321	250	2.224	2.357	2.356	250
2_u	$(^3\Pi_u)$	2.236	2.290	2.288	248	2.230	2.367	2.366	248	2.228	2.403	2.402	249
$1_u(2)$	$(^3\Pi_u)$	2.238	2.332	2.331	247	2.232	2.409	2.408	247	2.230	2.445	2.444	248
$0_u^+(1)$	$(^3\Pi_u)$	2.242	2.385	2.385	242	2.237	2.462	2.462	241	2.235	2.497	2.497	241
$0_u^-(2)$	$(^3\Pi_u)$	2.240	2.396	2.395	246	2.234	2.472	2.472	246	2.232	2.508	2.507	247
$0_g^+(2)$	$(^1\Sigma_g^+)$	2.235	2.501	2.499	245	2.229	2.573	2.572	245	2.227	2.607	2.606	247
$1_u(3)$	$(^1\Pi_u)$	2.247	2.619	2.620	240	2.241	2.694	2.695	240	2.239	2.729	2.729	241
$0_u^+(2)$	$(^1\Sigma_u^+)$	2.368	2.724	2.805	223	2.361	2.763	2.838	227	2.357	2.781	2.853	227

Table S6. Bond length (Å), harmony frequency (cm^{-1}), adiabatic excitation energy (eV), and vertical excitation energies (eV) of Ag_2 based on EOM-CCSD.

		TZ				QZ				5Z			
State		R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e
SR													
$^1\Sigma_g^+(1)$	$(1\sigma_g^+)^2$	2.546	0	0	189	2.537	0	0	191	2.538	0	0	191
$^3\Sigma_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	-	-	1.825	-	-	-	1.835	-	-	-	1.838	-
$^1\Sigma_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	2.682	2.907	2.975	148	2.675	2.930	2.993	149	2.677	2.936	3.000	148
$^3\Pi_u(1)$	$(1\sigma_g^+)^1\pi_u^1$	2.594	3.438	3.452	168	2.585	3.454	3.465	170	2.586	3.457	3.470	170
$^3\Sigma_g^+(1)$	$(1\sigma_g^+)^1(2\sigma_g^+)^1$	2.784	4.238	4.333	113	2.779	4.266	4.377	114	2.781	4.269	4.391	111
$^1\Pi_u(1)$	$(1\sigma_g^+)^1\pi_u^1$	2.646	4.463	4.500	147	2.638	4.483	4.517	149	2.641	4.487	4.522	148
$^3\Sigma_g^+(2)$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.556	4.479	4.484	260	2.527	4.558	4.557	251	2.518	4.593	4.594	258
$^1\Sigma_g^+(2)$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.555	4.591	4.591	131	2.589	4.654	4.660	111	2.625	4.675	4.687	107
$^3\Pi_u(2)$	$\pi_g^1(2\sigma_u^+)^1$	2.505	4.652	4.653	189	2.496	4.752	4.754	191	2.497	4.798	4.800	191
$^1\Sigma_g^+(3)$	$(1\sigma_g^+)^1(2\sigma_g^+)^1$	2.626	4.956	4.998	191	2.599	5.020	5.045	199	2.590	5.047	5.066	201
$^1\Pi_u(2)$	$\pi_g^1(2\sigma_u^+)^1$	2.527	4.976	4.974	186	2.515	5.068	5.068	188	2.515	5.111	5.110	187
SOC													
$0_g^+(1)$	$(^1\Sigma_g^+)$	2.547	0	0	189	2.538	0	0	191	2.539	0	0	191
$0_u^+(1)$	$(^3\Sigma_u^+)$	-	-	1.823	-	-	-	1.832	-	-	-	1.836	-
$1_u(1)$	$(^3\Sigma_u^+)$	-	-	1.823	-	-	-	1.832	-	-	-	1.836	-
$0_u^+(1)$	$(^1\Sigma_u^+)$	2.683	2.902	2.970	148	2.675	2.925	2.987	149	2.677	2.931	2.994	148
$0_u^-(2)$	$(^3\Pi_u)$	2.592	3.389	3.402	169	2.583	3.404	3.415	171	2.584	3.409	3.420	170
$0_u^+(2)$	$(^3\Pi_u)$	2.592	3.391	3.404	169	2.583	3.406	3.417	171	2.585	3.411	3.422	170
$1_u(2)$	$(^3\Pi_u)$	2.594	3.429	3.443	168	2.586	3.445	3.457	170	2.587	3.450	3.462	169
$2_u(1)$	$(^3\Pi_u)$	2.597	3.471	3.486	167	2.588	3.488	3.501	169	2.590	3.493	3.506	168
$0_g^-(1)$	$(^3\Sigma_g^+)$	2.785	4.227	4.319	112	2.780	4.255	4.365	114	2.782	4.259	4.379	111
$1_g(1)$	$(^3\Sigma_g^+)$	2.784	4.227	4.319	112	2.779	4.255	4.365	114	2.782	4.259	4.379	111
$1_u(3)$	$(^1\Pi_u)$	2.642	4.453	4.485	145	2.637	4.474	4.507	147	2.640	4.479	4.513	148
$0_g^-(2)$	$(^3\Sigma_g^+)$	2.565	4.458	4.467	252	2.536	4.537	4.537	242	2.525	4.572	4.573	250
$1_g(2)$	$(^3\Sigma_g^+)$	2.564	4.461	4.470	252	2.534	4.541	4.540	243	2.524	4.576	4.576	250
$2_u(2)$	$(^3\Pi_u)$	2.512	4.530	4.528	185	2.503	4.628	4.629	189	2.503	4.674	4.674	189
$0_g^+(2)$	$(^1\Sigma_g^+)$	2.560	4.567	4.567	137	2.586	4.632	4.638	119	2.616	4.655	4.667	111
$1_u(4)$	$(^3\Pi_u)$	2.528	4.608	4.607	195	2.512	4.702	4.702	189	2.511	4.746	4.746	188
$0_u^-(3)$	$(^3\Pi_u)$	2.520	4.737	4.735	180	2.510	4.835	4.835	183	2.511	4.881	4.881	182
$0_u^+(3)$	$(^3\Pi_u)$	2.514	4.749	4.747	184	2.505	4.848	4.848	187	2.506	4.893	4.893	186
$0_g^+(3)$	$(^1\Sigma_g^+)$	2.650	4.922	4.978	175	2.620	4.987	5.022	184	2.611	5.013	5.043	187
$1_u(5)$	$(^1\Pi_u)$	2.545	4.966	4.966	173	2.533	5.061	5.060	176	2.533	5.104	5.103	175

Table S7. Bond length (Å), harmony frequency (cm^{-1}), adiabatic excitation energy (eV), and vertical excitation energies (eV) of Au_2 based on EOM-CCSD.

		TZ				QZ				5Z			
State		R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e
SR													
$^1\sum_g^+$	$(1\sigma_g^+)^2$	2.493	0	0	187	2.490	0	0	188	2.488	0	0	188
$^3\sum_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	-	-	2.297	-	2.888	1.955	2.307	62	2.889	1.961	2.310	61
$^3\sum_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.478	2.344	2.341	185	2.474	2.421	2.418	186	2.471	2.454	2.452	186
$^3\prod_u$	$\pi_g^1(2\sigma_u^+)^1$	2.468	2.448	2.445	186	2.465	2.535	2.533	186	2.462	2.573	2.571	187
$^1\sum_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.485	2.842	2.840	180	2.481	2.915	2.913	181	2.478	2.946	2.944	181
$^1\sum_u^+$	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	2.617	2.933	3.048	155	2.613	2.970	3.080	156	2.611	2.985	3.092	156
$^1\prod_u$	$\pi_g^1(2\sigma_u^+)^1$	2.484	2.928	2.926	179	2.480	3.009	3.007	180	2.478	3.045	3.043	180
SOC													
$0_g^+(1)$		2.488	0	0	189	2.479	0	0	190	2.483	0	0	190
$0_u^+(1)$		2.786	1.941	2.157	75	2.783	1.972	2.186	75	2.793	1.965	2.194	73
$1_u(1)$		2.797	1.947	2.073	73	2.793	1.977	2.143	74	2.803	1.970	2.164	72
2_u		2.468	1.963	1.961	185	2.458	2.046	2.047	187	2.463	2.081	2.080	185
0_g^-		2.496	2.158	2.160	175	2.485	2.235	2.235	177	2.488	2.263	2.264	177
$1_u(2)$		-	-	2.245	-	2.521	2.245	2.278	255	2.518	2.268	2.294	245
1_g		2.494	2.170	2.171	176	2.482	2.246	2.247	178	2.486	2.275	2.275	178
$0_u^+(1)$		2.531	2.439	2.455	157	2.523	2.515	2.529	157	2.529	2.541	2.556	154
$0_g^+(2)$		2.514	2.608	2.616	163	2.501	2.683	2.688	166	2.504	2.709	2.714	167
$0_u^-(2)$		2.544	2.669	2.699	164	2.527	2.746	2.764	168	2.530	2.771	2.791	168
$1_u(3)$		2.547	2.910	2.936	151	2.531	2.989	3.007	154	2.536	3.016	3.036	155
$0_u^+(2)$		2.547	3.175	3.211	178	2.535	3.224	3.251	180	2.539	3.234	3.265	186

Table S8. Bond length (Å), harmony frequency (cm^{-1}), adiabatic excitation energy (eV), and vertical excitation energies (eV) of Rg_2 based on EOM-CCSD.

		TZ				QZ			
State		R_e	AEEs	VEEs	ω_e	R_e	AEEs	VEEs	ω_e
SR									
$^1\sum_g^+$	$(\pi_g)^4$	2.497	0	0	194	2.471	0	0	207
$^3\prod_u$	$\pi_g^1(2\sigma_u^+)^1$	2.554	0.196	0.202	170	2.520	0.231	0.210	184
$^1\prod_u$	$\pi_g^1(2\sigma_u^+)^1$	2.576	0.921	0.939	155	2.534	0.967	0.943	174
$^3\Delta_g$	$\delta_u^1(2\sigma_u^+)^1$	2.668	0.916	1.047	134	2.618	1.022	1.070	153
$^1\Delta_g$	$\delta_u^1(2\sigma_u^+)^1$	2.676	1.071	1.213	131	2.623	1.182	1.234	150
$^3\Delta_u$	$\delta_g^1(2\sigma_u^+)^1$	2.778	1.288	1.628	110	2.708	1.441	1.644	132
$^1\Delta_u$	$\delta_g^1(2\sigma_u^+)^1$	2.789	1.416	1.769	107	2.713	1.574	1.785	130
$^3\sum_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.615	1.901	1.966	157	2.579	1.926	1.934	171
$^1\sum_g^+$	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	2.649	2.157	2.262	142	2.603	2.196	2.227	158
SOC									
$0_g^+(1)$		2.550	0	0	152	2.515	0	0	171
$2_u(1)$		2.545	-0.593	-0.594	156	2.512	-0.575	-0.574	172
$1_u(1)$		2.557	-0.390	-0.388	146	2.519	-0.369	-0.369	165
3_g		2.649	-0.007	0.072	122	2.598	0.067	0.106	143
$2_g(1)$		2.646	0.047	0.122	122	2.595	0.121	0.156	143
$0_u^-(1)$		-	-	0.214	-	-	-	0.236	-
$1_u(2)$		2.892	0.181	0.553	123	2.830	0.334	0.567	114
3_u		2.816	0.411	0.716	84	2.722	0.545	0.744	111
$2_u(2)$		2.813	0.453	0.745	82	2.716	0.587	0.773	111
0_u^+		2.537	0.624	0.621	172	2.510	0.639	0.704	184
$2_g(2)$		-	-	1.352	-	2.879	1.031	1.361	66
$1_g(1)$		-	-	1.349	-	2.823	1.106	1.366	72
0_g^-		2.591	1.760	1.790	154	2.556	1.763	1.774	168
$1_g(2)$		2.594	1.822	1.855	154	2.560	1.832	1.842	168
$0_g^+(2)$		2.641	2.048	2.123	132	2.593	2.072	2.107	148

Table S9. Excitation energies (ΔE/eV), type assignments, NTO transitions, squared norm of doubles amplitudes (R_2), NTO participation ratio (PR_{NTO}), and the number of promoted electrons (p) of the first six lowed excited states of Cu_2 computed at EOMEE-CCSD/Aug-cc-pwcVQZ-PP level of theory.

State	ΔE	Type	Transition	R_2	PR_{NTO}	p
$^1\Sigma_g^+$	0	$(1\sigma_g^+)^2$	-	-	-	-
$^3\Sigma_u^+$	2.057	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.055	1.045	1.345
$^3\Sigma_g^+$	2.331	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.131	1.139	1.362
$^3\Pi_u$	2.427	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.131	1.193	1.384
$^1\Sigma_g^+$	2.586	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.139	1.137	1.541
$^1\Pi_u$	2.698	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.139	1.198	1.541
$^1\Sigma_u^+$	2.826	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.128	1.139	1.418

Table S10. Excitation energies (ΔE/eV), type assignments, NTO transitions, squared norm of doubles amplitudes (R_2), NTO participation ratio (PR_{NTO}), and the number of promoted electrons (p) of the first six lowed excited states of Ag_2 computed at EOMEE-CCSD/Aug-cc-pwcVQZ-PP level of theory.

State	ΔE	Type	Transition	R_2	PR_{NTO}	p
$^1\Sigma_g^+(1)$	0	$(1\sigma_g^+)^2$	-	-	-	-
$^3\Sigma_u^+$	1.835	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.053	1.028	1.296
$^1\Sigma_u^+$	2.993	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.124	1.028	1.309
$^3\Pi_u(1)$	3.465	$(1\sigma_g^+)^1\pi_u^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\pi_u,E}$	0.047	1.045	1.294
$^3\Sigma_g^+(1)$	4.377	$(1\sigma_g^+)^1(2\sigma_g^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_g,E}/\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.065	1.496	1.253
$^1\Pi_u(1)$	4.517	$(1\sigma_g^+)^1\pi_u^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\pi_u,E}$	0.088	1.045	1.321
$^3\Sigma_g^+(2)$	4.557	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}/\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_g,E}$	0.108	1.786	1.246
$^1\Sigma_g^+(2)$	4.660	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}/\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_g,E}$	0.106	1.496	1.341
$^3\Pi_u(2)$	4.754	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.122	1.134	1.282
$^1\Sigma_g^+(3)$	5.045	$(1\sigma_g^+)^1(2\sigma_g^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_g,E}/\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.169	1.786	1.333
$^1\Pi_u(2)$	5.068	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.132	1.134	1.388

Table S11. Excitation energies (ΔE/eV), type assignments, NTO transitions, squared norm of doubles amplitudes (R_2), NTO participation ratio (PR_{NTO}), and the number of promoted electrons (p) of the first six lowed excited states of Au_2 computed at EOMEE-CCSD/Aug-cc-pwcVQZ-PP level of theory.

State	ΔE	Type	Transition	R_2	PR_{NTO}	p
$^1\Sigma_g^+$	0	$(1\sigma_g^+)^2$	-	-	-	-
$^3\Sigma_u^+$	2.307	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.069	1.039	1.293
$^3\Sigma_g^+$	2.418	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.106	1.063	1.278
$^3\Pi_u$	2.533	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.109	1.075	1.273
$^1\Sigma_g^+$	2.913	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.122	1.063	1.366
$^1\Pi_u$	3.007	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.123	1.049	1.371
$^1\Sigma_u^+$	3.080	$(1\sigma_g^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_g,H}\rightarrow\psi_{\sigma_u,E}$	0.121	1.111	1.291

Table S12. Excitation energies (ΔE/eV), type assignments, NTO transitions, squared norm of doubles amplitudes (R_2), NTO participation ratio (PR_{NTO}), and the number of promoted electrons (p) of the first eight lowed excited states of Rg_2 computed at EOMEE-CCSD/PVQZ-SC level of theory.

State	ΔE	Type	Transition	R_2	PR_{NTO}	p
$^1\Sigma_g^+$	0	$(\pi_g)^4$	-	-	-	-
$^3\Pi_u$	0.210	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.102	1.035	1.286
$^1\Pi_u$	0.943	$\pi_g^1(2\sigma_u^+)^1$	$\psi_{\pi_g,H}\rightarrow\psi_{\sigma_u,E}$	0.119	1.024	1.287
$^3\Delta_g$	1.070	$\delta_u^1(2\sigma_u^+)^1$	$\psi_{\delta_u,H}\rightarrow\psi_{\sigma_u,E}$	0.111	1.029	1.300
$^1\Delta_g$	1.234	$\delta_u^1(2\sigma_u^+)^1$	$\psi_{\delta_u,H}\rightarrow\psi_{\sigma_u,E}$	0.125	1.024	1.298
$^3\Delta_u$	1.644	$\delta_g^1(2\sigma_u^+)^1$	$\psi_{\delta_g,H}\rightarrow\psi_{\sigma_u,E}$	0.115	1.039	1.299
$^1\Delta_u$	1.785	$\delta_g^1(2\sigma_u^+)^1$	$\psi_{\delta_g,H}\rightarrow\psi_{\sigma_u,E}$	0.131	1.032	1.296
$^3\Sigma_g^+$	1.934	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.090	1.033	1.288
$^1\Sigma_g^+$	2.227	$(1\sigma_u^+)^1(2\sigma_u^+)^1$	$\psi_{\sigma_u,H}\rightarrow\psi_{\sigma_u,E}$	0.121	1.023	1.284