The electronic supplementary information for

Coinage metalides: a new type of excess electron compounds with high stability and large nonlinear optical responses

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1. Tables

Table S1 The symmetry, the distance between Li^+ and Cu^- ($d_{Li\text{-}Cu}$, in Å), Li^+-F distance ($d_{Li\text{-}F}$, in Å), and distance between Cu^- and H ($d_{Cu\text{-}H}$, in Å) for Li^+-**1**-Cu^- optimized by using the same LANL2DZ basis set for Cu and different basis sets for Li, C, H, and F atoms.

Basis sets	Symmetry	$d_{Li\text{-}Cu}$	$d_{Li\text{-}F}$	$d_{Cu\text{-}H}$
6-31G	C_{3v}	6.150	1.826	2.518
6-31G(d)	C_{3v}	6.124	1.821	2.597
6-31+G(d)	C_{3v}	6.162	1.844	2.591
6-31+G(d, p)	$\boldsymbol{C_{3v}}$	**6.147**	**1.847**	**2.574**
6-31++G(d, p)	C_{3v}	6.147	1.848	2.575
6-311+G(d)	C_{3v}	6.189	1.854	2.588
6-311+G(d, p)	C_{3v}	6.182	1.852	2.583
6-311++G(d, p)	C_{3v}	6.185	1.852	2.586
6-311++G(2d, 2p)	C_{3v}	6.151	1.843	2.583
6-311++G(3df, 3pd)	$\boldsymbol{C_{3v}}$	**6.128**	**1.842**	**2.572**

Table S2 The symmetry, the distance between Li^+ and Cu^- ($d_{Li\text{-}Cu}$, in Å), Li^+-F distance ($d_{Li\text{-}F}$, in Å), and distance between Cu^- and H ($d_{Cu\text{-}H}$, in Å) for Li^+-**1**-Cu^- optimized by using the same 6-31+G(d, p) basis set for Li, C, H, and F atoms and different basis sets for Cu atom.

Basis sets	Symmetry	$d_{Li\text{-}Li}$	$d_{Li\text{-}F}$	$d_{Cu\text{-}H}$
LANL2DZ	C_{3v}	6.176	1.847	2.602
SDD	C_{3v}	6.176	1.847	2.602
Def2-TZVP	C_{3v}	6.217	1.846	2.638
aug-cc-pVDZ-pp	$\boldsymbol{C_{3v}}$	**6.192**	**1.847**	**2.615**
aug-cc-pVTZ-pp	C_{3v}	6.206	1.847	2.626
aug-cc-pVQZ-pp	$\boldsymbol{C_{3v}}$	**6.197**	**1.846**	**2.621**

Table S3 The dipole moments (μ_0, in au), polarizabilities (α_0, in au), first hyperpolarizabilities (β_0, in au) of Li^+-**1**-Cu^- calculated by using the same LANL2DZ basis set for Cu and different basis sets for Li, C, H, and F atoms.

Basis sets	μ_0	α_0	β_0
6-31G	4.210	191	10477
6-31G(d)	4.731	204	16291
6-31+G(d)	**4.474**	**203**	**16762**
6-31+G(d, p)	4.467	203	16245
6-31++G(d, p)	4.458	203	16419
6-311+G(d, p)	4.375	202	15772
6-311++G(d, p)	4.373	201	15315
6-311++G(2d, 2p)	4.478	204	16379
6-311++G(3df, 3pd)	**4.515**	**205**	**16619**

Table S4 The dipole moments (μ_0, in au), polarizabilities (α_0, in au), first hyperpolarizabilities (β_0, in au) of Li^+-**1**-Cu^- calculated by using the same 6-31+G(d) basis set for Li, C, H, and F atoms and different basis sets for Cu atom.

Basis sets	$d_{Li\text{-}Li}$	$d_{Li\text{-}F}$	$d_{Li\text{-}H}$
LANL2DZ	4.499	211	20744
SDD	4.522	202	15832
Def2-TZVP	4.426	202	23078
aug-cc-pVDZ-pp	4.515	205	16619
aug-cc-pVTZ-pp	**4.466**	**213**	**11858**
aug-cc-pVQZ-pp	**4.470**	**211**	**12537**

2. Figures

Fig. S1 The optimized equilibrium structure of the **1** molecule.

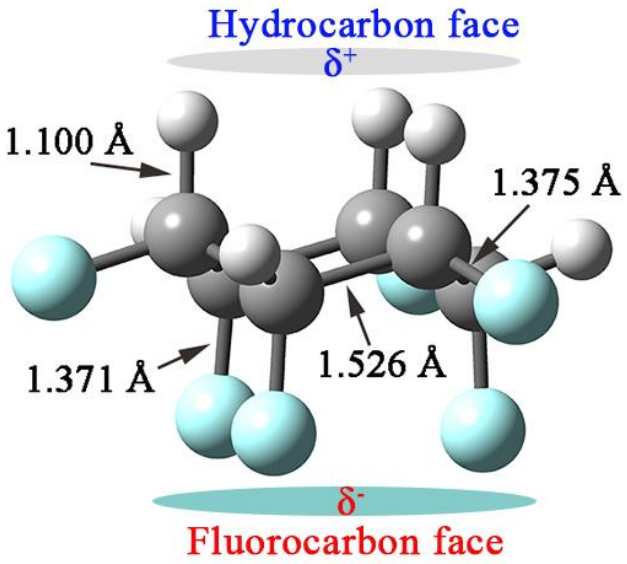


Fig. S2 Isosurface maps of α_{zz} density $-z\rho_z(\mathbf{r})$ for M^+-**1**-M'^- (M = Li, Na, and K; M' = Cu, Ag, and Au) with the same isovalue of 0.3, where green and blue surfaces denote positive and negative densities, respectively.

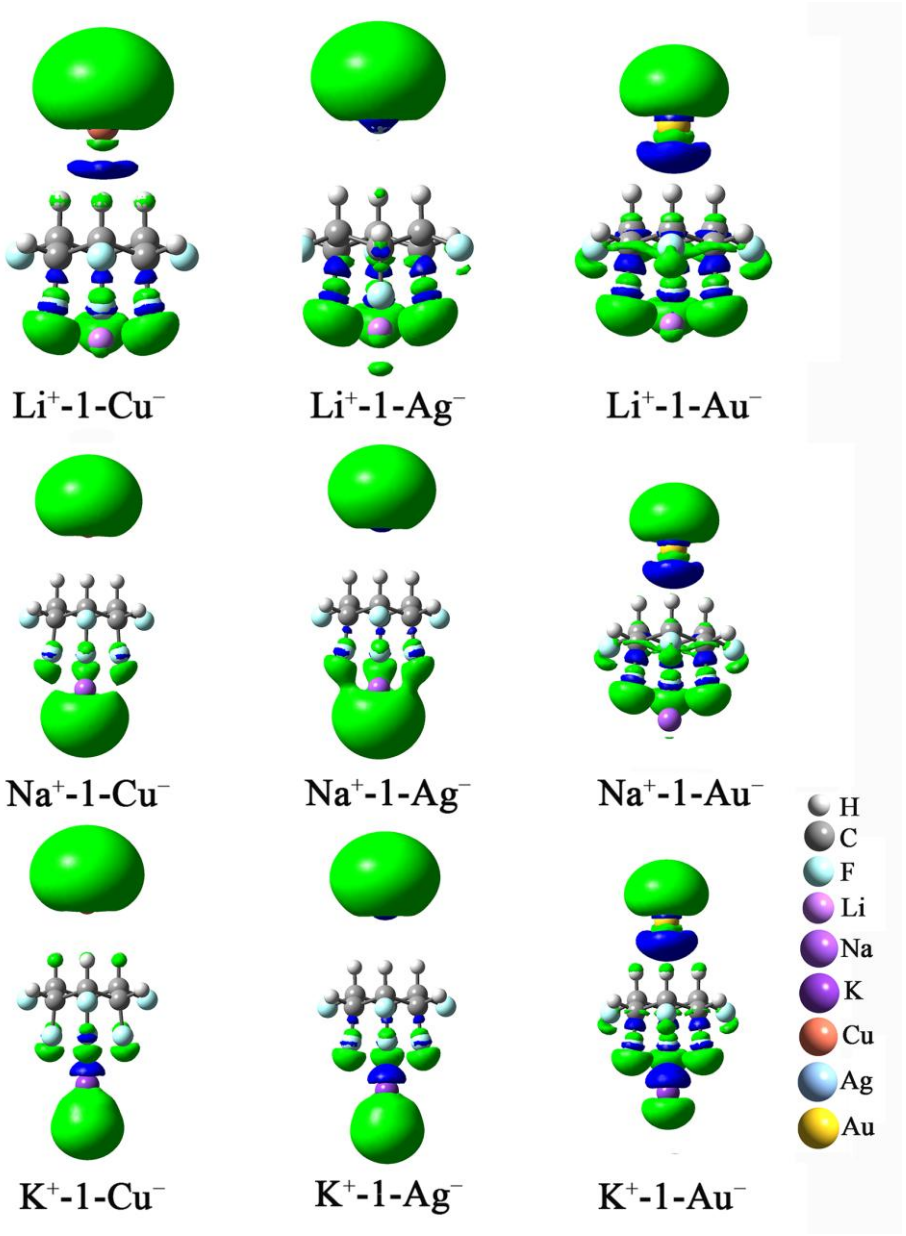
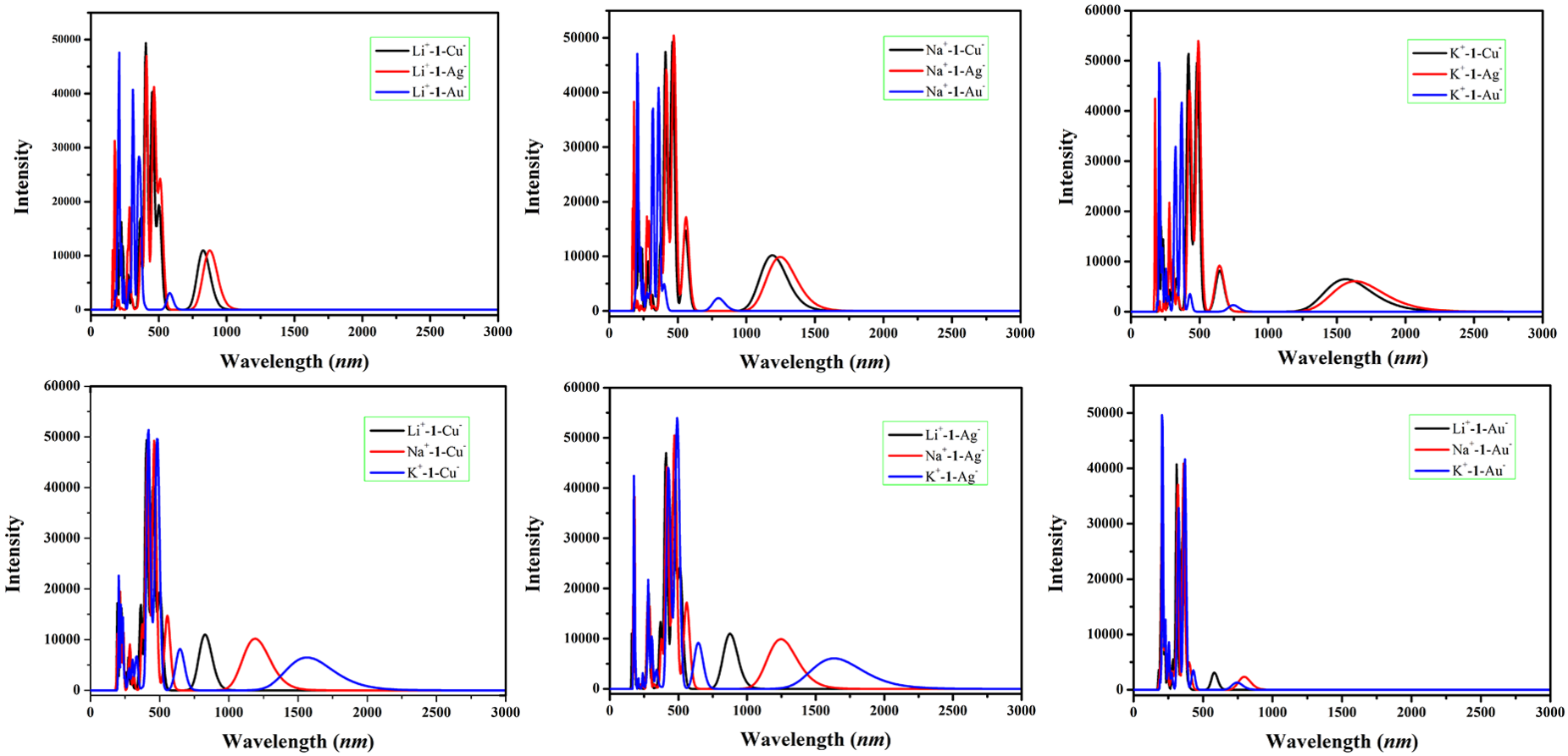


Fig. S3 The ultraviolet-visible-infrared absorption spectra of M^{+}-**1**-M'^{-} (M = Li, Na, and K; M' = Cu, Ag, and Au).



3. Cartesian coordinates

a. The Cartesian coordinates of Li-1-Cu with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	0.000000	1.424600	-0.156900
C	1.260600	0.727800	-0.605800
C	1.233700	-0.712300	-0.156900
C	-0.000000	-1.455600	-0.605800
C	-1.233700	-0.712300	-0.156900
C	-1.260600	0.727800	-0.605800
H	2.153400	1.243300	-0.245300
H	0.000000	1.397400	0.964900
H	-0.000000	-2.486500	-0.245300
H	-1.210200	-0.698700	0.964900
H	-2.153400	1.243300	-0.245300
H	1.210200	-0.698700	0.964900
F	-0.000000	-1.569400	-2.042200
F	1.359100	0.784700	-2.042200
F	-1.359100	0.784700	-2.042200
F	0.000000	2.726100	-0.600000
F	-2.360800	-1.363000	-0.600000
F	2.360800	-1.363000	-0.600000
Li	0.000000	0.000000	-3.015000
Cu	0.000000	0.000000	3.170800

b. The Cartesian coordinates of Li-1-Ag with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	0.000000	1.429500	-0.582900
C	1.261500	0.728300	-1.028700
C	1.238000	-0.714700	-0.582900
C	-0.000000	-1.456700	-1.028700
C	-1.238000	-0.714700	-0.582900
C	-1.261500	0.728300	-1.028700
H	2.155000	1.244200	-0.670100
H	0.000000	1.422000	0.535300
H	-0.000000	-2.488400	-0.670100
H	-1.231500	-0.711000	0.535300
H	-2.155000	1.244200	-0.670100
H	1.231500	-0.711000	0.535300
F	0.000000	-1.565500	-2.463100
F	1.355800	0.782800	-2.463100
F	-1.355800	0.782800	-2.463100
F	0.000000	2.723800	-1.046400
F	-2.358800	-1.361900	-1.046400
F	2.358800	-1.361900	-1.046400

Li	0.000000	0.000000	-3.444600
Ag	0.000000	0.000000	2.861800

c. The Cartesian coordinates of Li-1-Au with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	-0.000000	1.440800	-0.973600
C	1.263000	0.729200	-1.411300
C	1.247800	-0.720400	-0.973600
C	0.000000	-1.458300	-1.411300
C	-1.247800	-0.720400	-0.973600
C	-1.263000	0.729200	-1.411300
H	2.157600	1.245700	-1.058900
H	-0.000000	1.454100	0.138600
H	0.000000	-2.491400	-1.058900
H	-1.259300	-0.727000	0.138600
H	-2.157600	1.245700	-1.058900
H	1.259300	-0.727000	0.138600
F	0.000000	-1.557400	-2.845100
F	1.348700	0.778700	-2.845100
F	-1.348700	0.778700	-2.845100
F	-0.000000	2.719100	-1.487900
F	-2.354800	-1.359600	-1.487900
F	2.354800	-1.359600	-1.487900
Li	0.000000	0.000000	-3.824700
Au	0.000000	0.000000	2.204500

d. The Cartesian coordinates of Na-1-Cu with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	-1.235500	0.713300	0.045300
C	0.000000	1.461900	-0.397000
C	1.235500	0.713300	0.045300
C	1.266000	-0.731000	-0.397000
C	-0.000000	-1.426600	0.045300
C	-1.266000	-0.731000	-0.397000
H	0.000000	2.481700	-0.003300
H	-1.227800	0.708900	1.162900
H	2.149200	-1.240900	-0.003300
H	-0.000000	-1.417800	1.162900
H	-2.149200	-1.240900	-0.003300
H	1.227800	0.708900	1.162900
F	1.392000	-0.803700	-1.814400
F	0.000000	1.607300	-1.814400
F	-1.392000	-0.803700	-1.814400
F	-2.360300	1.362700	-0.413900

F	-0.000000	-2.725400	-0.413900
F	2.360300	1.362700	-0.413900
Na	0.000000	0.000000	-3.279200
Cu	0.000000	0.000000	3.416800

e. The Cartesian coordinates of Na-1-Ag with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	0.000000	1.430600	-0.378400
C	1.266800	0.731400	-0.817000
C	1.238900	-0.715300	-0.378400
C	-0.000000	-1.462800	-0.817000
C	-1.238900	-0.715300	-0.378400
C	-1.266800	0.731400	-0.817000
H	2.150400	1.241500	-0.424600
H	0.000000	1.437500	0.736700
H	-0.000000	-2.483100	-0.424600
H	-1.244900	-0.718700	0.736700
H	-2.150400	1.241500	-0.424600
H	1.244900	-0.718700	0.736700
F	0.000000	-1.605600	-2.233800
F	1.390500	0.802800	-2.233800
F	-1.390500	0.802800	-2.233800
F	0.000000	2.723100	-0.854200
F	-2.358200	-1.361500	-0.854200
F	2.358200	-1.361500	-0.854200
Na	0.000000	0.000000	-3.704700
Ag	0.000000	0.000000	3.078900

f. The Cartesian coordinates of Na-1-Au with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	-0.000000	1.440700	-0.797600
C	1.269600	0.733000	-1.226200
C	1.247700	-0.720400	-0.797600
C	0.000000	-1.466000	-1.226200
C	-1.247700	-0.720400	-0.797600
C	-1.269600	0.733000	-1.226200
H	2.152200	1.242600	-0.832600
H	-0.000000	1.465600	0.312600
H	0.000000	-2.485100	-0.832600
H	-1.269200	-0.732800	0.312600
H	-2.152200	1.242600	-0.832600
H	1.269200	-0.732800	0.312600
F	0.000000	-1.611500	-2.642900
F	1.395600	0.805800	-2.642900

F	-1.395600	0.805800	-2.642900
F	-0.000000	2.718700	-1.318900
F	-2.354400	-1.359300	-1.318900
F	2.354400	-1.359300	-1.318900
Au	0.000000	0.000000	2.405200
Na	0.000000	0.000000	-4.095700

g. The Cartesian coordinates of K-1-Cu with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	-1.237400	0.714400	0.287100
C	-0.000000	1.463600	-0.153500
C	1.237400	0.714400	0.287100
C	1.267500	-0.731800	-0.153500
C	-0.000000	-1.428800	0.287100
C	-1.267500	-0.731800	-0.153500
H	0.000000	2.479700	0.251400
H	-1.241100	0.716500	1.401400
H	2.147500	-1.239900	0.251400
H	-0.000000	-1.433100	1.401400
H	-2.147500	-1.239900	0.251400
H	1.241100	0.716500	1.401400
F	1.396800	-0.806400	-1.561400
F	0.000000	1.612900	-1.561400
F	-1.396800	-0.806400	-1.561400
F	-2.359300	1.362200	-0.186700
F	-0.000000	-2.724300	-0.186700
F	2.359300	1.362200	-0.186700
K	0.000000	0.000000	-3.519000
Cu	0.000000	0.000000	3.679200

h. The Cartesian coordinates of K-1-Ag with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	0.000000	1.432100	-0.145800
C	1.267900	0.732000	-0.583900
C	1.240200	-0.716100	-0.145800
C	-0.000000	-1.464100	-0.583900
C	-1.240200	-0.716100	-0.145800
C	-1.267900	0.732000	-0.583900
H	2.148100	1.240200	-0.179800
H	0.000000	1.450200	0.966200
H	-0.000000	-2.480500	-0.179800
H	-1.255900	-0.725100	0.966200
H	-2.148100	1.240200	-0.179800
H	1.255900	-0.725100	0.966200

F	0.000000	-1.609600	-1.991200
F	1.393900	0.804800	-1.991200
F	-1.393900	0.804800	-1.991200
F	0.000000	2.722300	-0.633200
F	-2.357600	-1.361200	-0.633200
F	2.357600	-1.361200	-0.633200
K	0.000000	0.000000	-3.954400
Ag	0.000000	0.000000	3.335500

i. The Cartesian coordinates of K-1-Au with C_{3v} symmetry optimized at the M06-2X/6-31+G(d,p)&aug-cc-pVDZ-pp level.

C	-0.000000	1.441100	-0.590400
C	1.270600	0.733600	-1.018500
C	1.248000	-0.720500	-0.590400
C	0.000000	-1.467200	-1.018500
C	-1.248000	-0.720500	-0.590400
C	-1.270600	0.733600	-1.018500
H	2.149200	1.240900	-0.611400
H	-0.000000	1.476300	0.517300
H	0.000000	-2.481700	-0.611400
H	-1.278500	-0.738100	0.517300
H	-2.149200	1.240900	-0.611400
H	1.278500	-0.738100	0.517300
F	0.000000	-1.619500	-2.425700
F	1.402500	0.809700	-2.425700
F	-1.402500	0.809700	-2.425700
F	-0.000000	2.718300	-1.118700
F	-2.354100	-1.359200	-1.118700
F	2.354100	-1.359200	-1.118700
Au	0.000000	0.000000	2.630600
K	0.000000	0.000000	-4.361900