

## Nanoparticles and atoms geometro-wave potential unified and predicted properties

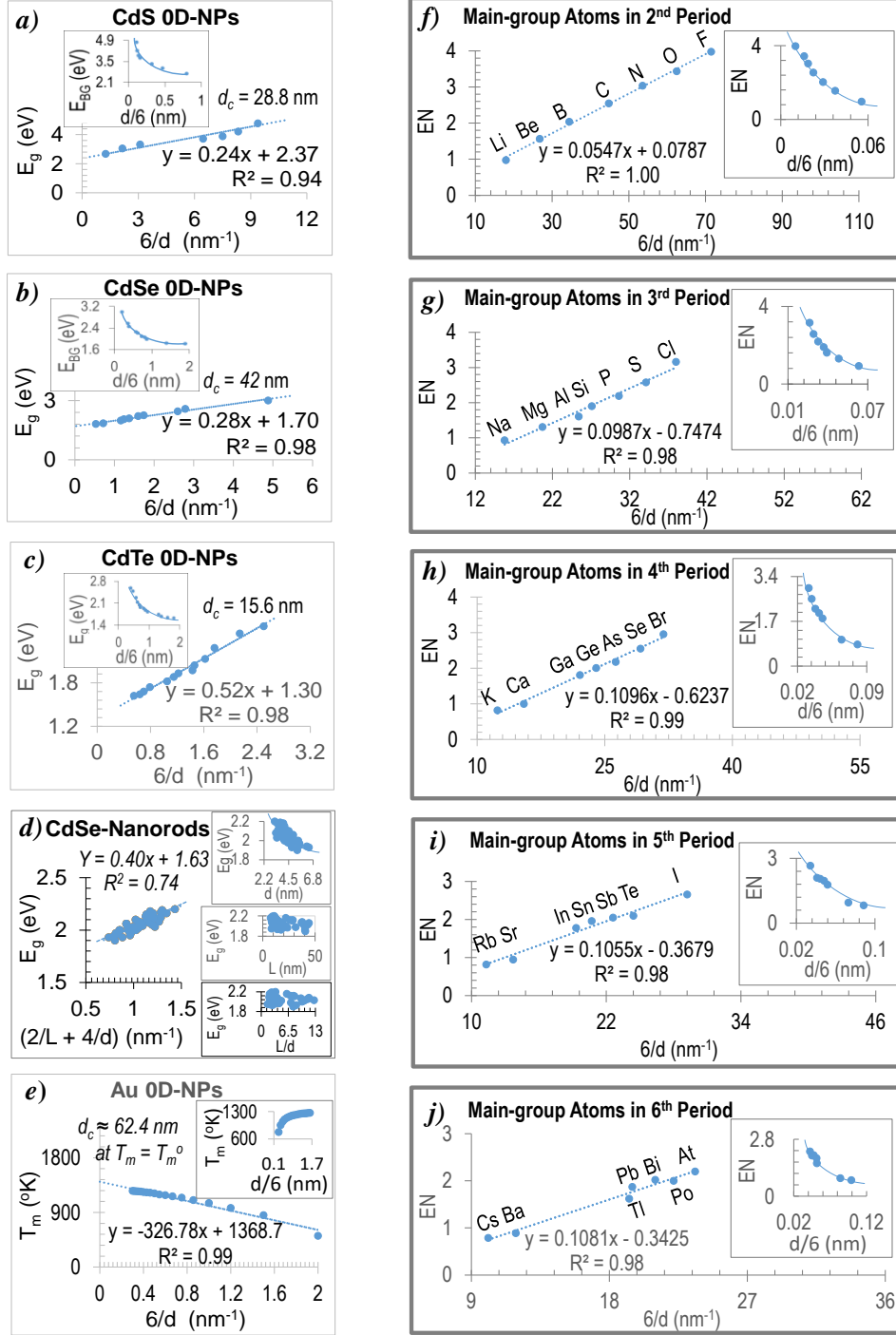
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**This work has introduced a geometrowave (GW) potential to linearly fit, consistently unify, and quantitatively predict and compare small particles' geometry-based properties known and new, which complements de Broglie's mass-based matter wave<sup>1</sup>. The “known” properties cover gold nanoparticles' (NPs') melting point and surface plasmon resonance, semiconducting NPs' optical bandgap, and main-group atoms' electronegativity (EN), ionization potential (IPs), and polarizability. The new properties include NP-surface atoms' layering (like atom-surface electrons'), self-assembled NPs' inter-bonding via sharing surface-atoms (like surface electron-shared interatomic bonding), and atom-like NPs GW-potential's periodicity like atoms electronegativity's.**

For all zero-dimensional (0D), 1D-, 2D-, and 3D-particles, let's quantize their geometry-based Surface Area-to-Volume (SA/V) ratio in the unit of (length<sup>-1</sup>) (see the **Extended Data Table S1**) to a geometro-wavenumber ( $\tilde{\nu}_{GW}$ ), and their (V/SA) ratio in the unit of (length) to a geometro-wavelength ( $\lambda_{GW}$ ), respectively. Thus, the geometro-wave potential (i.e. energy)  $\mu_{GW} = hc \cdot \tilde{\nu}_{GW} = hc / \lambda_{GW}$ ,

where the  $c$  = speed of light,  $h$  = Planck constant, and  $hc \approx 1.24$  (keV·nm). The  $\mu_{GW}$  is useful (see below) to prove that the pm- and nm-scales particles' long-thought “size-dependent” properties are all  $\mu_{GW}$ -dependent hence geometry-quantized.

For Cd-X (X = S, Se, Te) semiconductors, for example, their 0D-NPs' optical bandgap energies ( $E_g$ ) (see the **Extended Data Table S2**)<sup>2-5</sup> fit with their



**Fig. 1. Linear fits of  $\tilde{\nu}_{GW}$ .** With the  $E_g$  of Cd-chalcogenides NPs (a)-(d),  $T_m$  of Au-0D-NPs (e), and EN of main-group atoms in periods (f)-(j).

$\tilde{\nu}_{GW}$  (i.e.  $\mu_{GW}/hc$ ) values linearly (Figs. 1a-1c) and with their  $\lambda_{GW}$  (i.e.  $hc/\mu_{GW}$ ) values

curvedly (see the insets). From the linear equations, every intercept  $\approx E_{g(\text{bulk})}$ <sup>6</sup>. Further,

the trend of these linear slopes (i.e.  $0.24_{(\text{CdS-NP})} < 0.28_{(\text{CdS-NP})} < 0.52_{(\text{CdS-NP})}$ ) matches that of their  $E_{\text{g(Bulk)}}$  values<sup>6</sup> {i.e.  $2.42_{(\text{CdS})} > 1.74_{(\text{CdSe})} > 1.50_{(\text{CdTe})}$  (eV)}, and that of their EN<sup>7,8</sup>-based bond polarities  $\text{Cd-S} > \text{Cd-Se} > \text{Cd-Te}$ . Convincingly, the scattering  $E_{\text{g}}$  data<sup>9</sup> of CdSe-nanorods fit quite linearly (**Fig. 1d**) with their  $\tilde{\nu}_{\text{GW}}$  values (see the **Extended Data Table S3**), proving the generally applicable  $\mu_{\text{GW}}$  selective interaction with  $\lambda_{\text{photon}}$ . Likewise, the Au-0D-NPs' melting points<sup>10</sup> ( $T_{\text{m}}$ ) (see the **Extended Data Table S4**) fit linearly with their  $\tilde{\nu}_{\text{GW}}$  values (**Fig. 1e**) and curvedly with their  $\lambda_{\text{GW}}$  values (the inset), showing the intercept (1368.7 °K) that's 2.3% off the  $T_{\text{m(bulk)}}$  (1337.3 °K)<sup>3</sup>. The smaller NP's lower  $T_{\text{m}}$  reflects its surface atoms' lower activation energy that matches a longer electromagnetic (EM) wavelength ( $\lambda_{(\text{infrared})}$ ) with the NP's higher  $\mu_{\text{GW}}$ .

Further, the 0D-Au-NPs' surface plasmon resonance (SPR) wavelengths ( $\lambda_{\text{SPR}}$ )<sup>10</sup> and the main-group atoms'

polarizability<sup>8</sup> (see the **Extended Data Tables S5-S6**) fit linearly with their  $\lambda_{\text{GW}}$  (see the **Extended Data Fig. S1**) and curvedly with their  $\tilde{\nu}_{\text{GW}}$  values<sup>11</sup> (see two representative insets), respectively. This proves that the  $\mu_{\text{GW}}$  governs the particles' surface electrons movement.

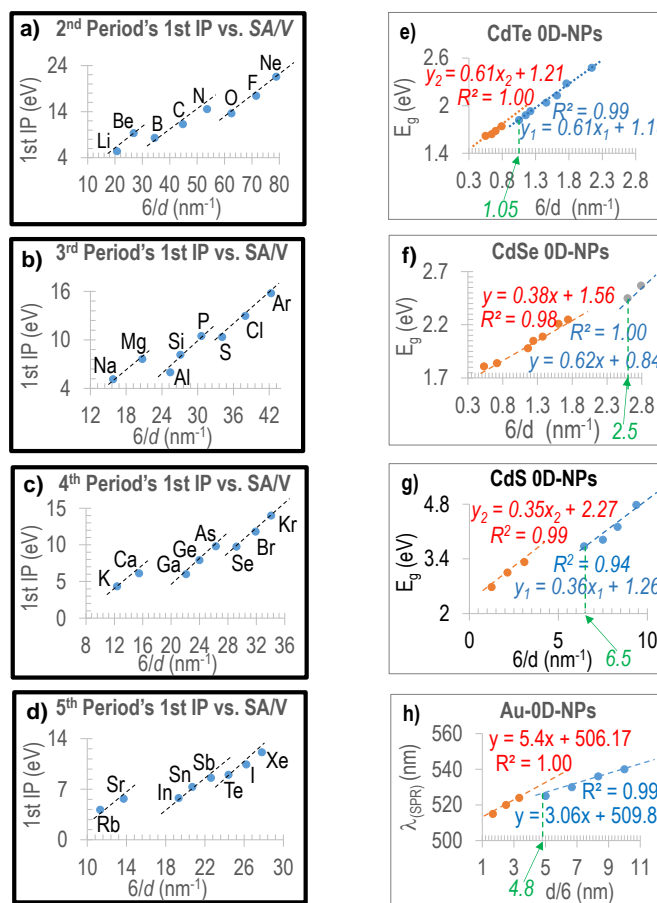
Consistently, every period of main-group atoms' Pauling EN data<sup>7</sup> fit linearly (**Fig. 1, f-j**) with their  $\tilde{\nu}_{\text{GW}}$  and curvedly (the insets) with their  $\lambda_{\text{GW}}$  values<sup>11</sup> (see the **Extended Data Table S6**). The gap between *s*- and *p*-orbitals increases from **Fig. 1g** to **Fig. 1j** for facilitating the *d*- and *f*-blocks atoms (omitted here for clarity) support all atoms'  $E_{\text{GW}}$ -quantified and electronegativity (EN)-complemented periodicities (**Table 1**), thus-revealing the atoms' and NPs' surface-layering properties below.

First, main-group atoms'  $\tilde{\nu}_{\text{GW}}$  values and first ionization potentials (or 1<sup>st</sup> IPs, in Mulliken's EN<sup>12</sup>, see the **Extended Data Table S6**) have indeed quantified the atom-

Table 1. Periodicities of Atoms $\tilde{\nu}_{GW}$																	
H 0.106 <b>56.6</b> 2.20																	He 0.062 <b>96.8</b>
Li 0.234 <b>20.6</b> 0.98	Be 0.224 <b>26.8</b> 1.57											B 0.174 <b>34.5</b> 2.04	C 0.134 <b>44.8</b> 2.55	N 0.112 <b>53.6</b> 3.04	O 0.096 <b>62.5</b> 3.44	F 0.084 <b>71.4</b> 3.98	Ne 0.076 <b>78.9</b>
Na 0.380 <b>15.8</b> 0.93	Mg 0.290 <b>20.7</b> 1.31											Al 0.236 <b>25.4</b> 1.61	Si 0.222 <b>27.0</b> 1.90	P 0.196 <b>30.6</b> 2.19	S 0.176 <b>34.1</b> 2.58	Cl 0.158 <b>38.0</b> 3.16	Ar 0.142 <b>42.3</b>
K 0.486 <b>12.3</b> 0.82	Ca 0.388 <b>15.5</b> 1.00	Sc 0.368 <b>16.3</b> 1.36	Ti 0.352 <b>17.0</b> 1.54	V 0.342 <b>17.5</b> 1.63	Cr 0.332 <b>18.1</b> 1.66	Mn 0.322 <b>18.6</b> 1.55	Fe 0.312 <b>19.2</b> 1.83	Co 0.304 <b>19.7</b> 1.88	Ni 0.298 <b>20.1</b> 1.91	Cu 0.290 <b>20.7</b> 1.90	Zn 0.282 <b>21.3</b> 1.65	Ga 0.272 <b>22.1</b> 1.81	Ge 0.250 <b>24.0</b> 2.01	As 0.228 <b>26.3</b> 2.18	Se 0.206 <b>29.1</b> 2.55	Br 0.188 <b>31.9</b> 2.96	Kr 0.176 <b>34.1</b>
Rb 0.530 <b>11.3</b> 0.82	Sr 0.438 <b>13.7</b> 0.95	Y 0.424 <b>14.2</b> 1.22	Zr 0.412 <b>14.7</b> 1.33	Nb 0.396 <b>15.2</b> 1.6	Mo 0.380 <b>15.8</b> 2.16	Tc 0.366 <b>16.4</b> 2.10	Ru 0.356 <b>16.9</b> 2.2	Rh 0.346 <b>17.3</b> 2.28	Pd 0.338 <b>17.8</b> 2.20	Ag 0.330 <b>18.2</b> 1.93	Cd 0.322 <b>18.6</b> 1.69	In 0.312 <b>19.2</b> 1.78	Sn 0.290 <b>20.7</b> 1.96	Sb 0.266 <b>22.6</b> 2.05	Te 0.246 <b>24.4</b> 2.1	I 0.230 <b>26.1</b> 2.66	Xe 0.216 <b>27.8</b> 2.60
Cs 0.596 <b>10.1</b> 0.79	Ba 0.506 <b>11.9</b> 0.89	La 0.390 <b>15.4</b> 1.10	Hf 0.416 <b>14.4</b> 1.3	Ta 0.400 <b>15.0</b> 1.5	W 0.386 <b>15.5</b> 1.7	Re 0.376 <b>16.0</b> 1.9	Os 0.370 <b>16.2</b> 2.2	Ir 0.360 <b>16.7</b> 2.2	Pt 0.354 <b>16.9</b> 2.2	Au 0.348 <b>17.2</b> 2.4	Hg 0.342 <b>17.5</b> 1.9	Tl 0.312 <b>15.8</b> 1.8	Pb 0.308 <b>19.5</b> 1.8	Bi 0.286 <b>21.0</b> 1.9	Po 0.270 <b>22.2</b> 2.0	At 0.300 <b>20.0</b> 2.2	Rn 0.240 <b>25.0</b>
		La 0.390 <b>15.4</b> 1.10	Ce 0.370 <b>16.2</b> 1.12	Pr 0.370 <b>16.2</b> 1.13	Nd 0.370 <b>16.2</b> 1.1	Pm 0.370 <b>16.2</b> 1.17	Sm 0.370 <b>16.2</b> 1.17	Eu 0.370 <b>16.7</b> 1.20	Gd 0.360 <b>17.1</b> 1.22	Tb 0.350 <b>17.1</b> 1.22	Dy 0.350 <b>17.1</b> 1.22	Ho 0.350 <b>17.1</b> 1.23	Er 0.350 <b>17.1</b> 1.24	Tm 0.350 <b>17.1</b> 1.25	Yb 0.350 <b>17.1</b> 1.25	Lu 0.350 <b>17.1</b> 1.0	
		Ac 0.390 <b>15.4</b> 1.1	Th 0.360 <b>16.7</b> 1.3	Pa 0.360 <b>16.7</b> 1.5	U 0.350 <b>17.1</b> 1.7	Np 0.350 <b>17.1</b> 1.3	Pu 0.350 <b>17.1</b> 1.3	Am 0.350 <b>17.1</b> 1.3	Cm 0.238 <b>25.2</b> 1.3	Bk 0.34 <b>17.6</b> 1.3	Cf 0.372 <b>16.1</b> 1.3	Es 0.372 <b>16.1</b> 1.3	Fm 0.334 <b>18.0</b> 1.3	Md 0.346 <b>17.3</b> 1.3	No 0.332 <b>18.1</b> 1.3	Lr 0.322 <b>18.1</b> 1.3	

surface electrons'  $\mu_{GW}$ -quantized layering in the  $s$ -orbital first and then  $p$ -orbitals before and after the half-fill (**Figs. 2a-2d**). The increasing gaps between the  $s$ - and  $p$ -orbitals (**Figs. 2b-2d**) match that in the **Figs. 1f-1j**. Further, the transition metals cations'  $\tilde{\nu}_{GW}$  fits linearly with the IP<sup>8</sup> (see the **Extended Data Table S7** and the **Extended Data Fig. S2**), showing the  $d$ -orbitals' negligible size change before and after the half-fill.

Likewise, zooming in the **Figs. 1a-1c** has revealed the NPs' sudden (i.e. quantized)  $E_g$  drop (see the green dash-lines) as CdTe-NP's (**Fig. 2e**) < CdSe-NP's (**Fig. 2f**) < CdS-NP's (**Fig. 2g**). This supports the PbSe-0D-NPs' negligible  $E_g$  drop (see the **Extended Data Table S8** and the **Extended Data Fig. S3**), since  $E_{g(\text{bulk-PbSe})} \approx 0.7 \text{ (eV)}^6 \ll E_{g(\text{bulk-CdTe})}$ . The  $E_g$  drop tells the NP-surface atoms'  $E_{GW}$ -quantized layering, somewhat like atom-surface electrons' (**Figs. 2a-2d**), revealing an



**Fig. 2.** Atoms' and NPs' structural layering from correlations of their  $\tilde{\nu}_{GW}$ . With main-group atoms 1<sup>st</sup> IP (a)-(d), with  $E_g$  for 0D-NPs of CdTe (e), CdSe (f), and CdS (g), and with Au-0D-NPs  $\lambda_{(SPR)}$  (h).

*Note: The green dash-line in (e)-(h) shows the start of the sudden drop in the  $E_g$  and  $\lambda_{(SPR)}$  values.*

atomistic nature<sup>13</sup> in smaller 0D-NPs' more blue-shifted  $E_g$ , which helps expand Bohr's atomic model (i.e. QM) to the 0D-NPs.

Further, zooming in the **Extended Data Fig. S1a** has disclosed the Au-0D-NPs' sudden drop of their ( $\lambda_{SPR}$ ) when  $\lambda_{GW} < 4.8$  (nm) (**Fig. 2h**), indicating that the Au-NPs'

surface atoms do layer like the Cd-X NPs' (**Figs. 2e-2g**).

The NPs' atomistic nature (**Figs. 2e-2h**) supports the smaller NPs' stronger inter-bonding (see the **Extended Data Fig. S4**) in self-assembly<sup>14-17</sup> and biomineralization<sup>18,19</sup> via sharing their surface atoms geometrically, like smaller atoms' stronger EN-based

bonding via sharing more surface electrons electromagnetically. This proves every NP behaving like a super atom, which helps expand the particle science.

In summary, the new geometro-wave potential has been proven generally useful to complement de Broglie's matter-wave (i.e. QM), and quantitatively predict and compare

and consistently unify the NPs and atoms geometry-quantized properties known and new. The new properties, including NPs' surface atoms layering, inter-NP bonding, and atoms'  $E_{GW}$ -generalized periodicity, have naturally helped derive new basics in physics, chemistry and chemical biology, which will be detailed separately.

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**Acknowledgement:** The author appreciates Drs. H. W. Kroto, J. T. Yates, Z. L. Wang, P. Pulay, C. D. Heyes, and H. C. Tian for fruitful discussions, and all friends and colleagues for supporting this four-year “big data” work.

## SUPPLEMENATRY DATA.

I. Extended Data Tables S1–S8.



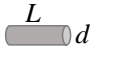
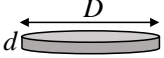
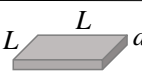



II. Extended Data Figures S1–S3.

## Nanoparticles and atoms geometro-wave potential unified and predicted properties

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### I. Extended Data Tables.

1). Extended Data Table S1.

Table S1. Simple-Shape Particles' $\tilde{\nu}_{GW}$ and Point Group of Symmetry					
	Shape	Surface-Area (SA)	Volume (V)	$\tilde{\nu}_{GW} (= SA/V)$	PntGrpSym
<b>0D</b>	 $d$	$\pi d^2$	$\pi d^3/6$	$(6/d)^*$	$R_3$
<b>1D</b>	 $L$ $d$	$4dL + 2d^2$	$d^2 L$	$(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$	$D_{2d}$
	 $L$ $d$	$\pi d^2/2 + \pi dL$	$\pi d^2 L/4$	$(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$	$D_{\infty d}$
<b>2D</b>	 $D$ $d$	$\pi D^2/2 + d\pi D$	$d\pi D^2/4$	$2/d + 4/D;$ or $2/d$ if $d \ll D$	$D_{\infty d}$
	 $L$ $L$ $d$	$2(aL + aL + L^2)$	$aL^2$	$2/d + 2/L + 2/L;$ or $2/d$ if $d \ll L$	$D_{4d}$
<b>3D</b>	 $d$	$6d^2$	$d^3$	$(6/d)^*$	$O_h$
	 $d$	$2 \times 3^{1/2} d^2$	$2^{1/2} d^3/3$	$3 \times 6^{1/2}/d$	$O_h$
	 $d$	$1.732d^2$	$0.118d^3$	$14.678/d$	$T_d$

\*The spherical and cubic particles share the same  $\tilde{\nu}_{GW}$  formula;  
 \*\*The two 1D-particles share the same  $\tilde{\nu}_{GW}$  formula.

2). Extended Data Table S2.

<b>Table S2. Semiconducting 0D-NPs <math>E_g</math> and <math>\tilde{\nu}_{GW}</math></b>								
<b>(a). CdS 0D-NP</b>			<b>(b). CdSe 0D-NP</b>			<b>(c). CdTe 0D-NP</b>		
$E_{BG}$ (eV)	d/6 (nm)	6/d (nm <sup>-1</sup> )	$E_{BG}$ (eV)	d/6 (nm)	6/d (nm <sup>-1</sup> )	$E_{BG}$ (eV)	d/6 (nm)	6/d (nm <sup>-1</sup> )
4.78	0.11	9.4	3.00	0.205	4.9	2.58	0.4	2.5
4.22	0.12	8.3	2.57	0.358	2.8	2.48	0.47	2.1
3.89	0.14	7.5	2.45	0.393	2.6	2.28	0.57	1.8
3.72	0.16	6.5	2.25	0.575	1.7	2.13	0.62	1.6
3.32	0.32	3.1	2.21	0.624	1.6	2.04	0.68	1.5
3.05	0.47	2.1	2.09	0.727	1.4	1.97	0.71	1.4
2.68	0.80	1.3	2.05	0.807	1.2	1.93	0.82	1.2
			1.98	0.860	2.2	1.88	0.87	1.2
			1.84	1.39	0.72	1.82	0.95	1.1
			1.61	1.88	0.53	1.74	1.3	0.79
						1.68	1.4	0.70
						1.64	1.6	0.64
						1.62	1.8	0.55

3). Extended Data Table S3.

<b>Table S3. Au-0D-NPs melting points and <math>\tilde{\nu}_{GW}</math></b>					
d/6 (nm)	6/d (nm <sup>-1</sup> )	$T_m$ (°K)	d/6 (nm)	6/d (nm <sup>-1</sup> )	$T_m$ (°K)
0.30	3.330	773	1.05	5.714	1223
0.38	15.79	953	1.13	5.301	1233
0.47	12.77	1043	1.22	4.918	1243
0.55	10.91	1098	1.30	4.615	1251
0.64	9.375	1138	1.38	4.349	1255
0.72	8.333	1163	1.45	4.138	1256
0.80	7.500	1183	1.53	3.922	1262
0.88	6.818	1198	1.62	3.704	1266
0.95	6.316	1208			

4). Extended Data Table S4.

Table S4. Semiconducting CdSe-Nanorod $E_g$ and $\tilde{\nu}_{GW}$									
$E_g$ (eV)	d (nm)	L (nm)	L/d	(SA/V)* (nm <sup>-1</sup> )	$E_g$ (eV)	d (nm)	L (nm)	L/d	(SA/V)* (nm <sup>-1</sup> )
2.20	3.2	11.0	3.4	1.4	2.07	4.3	8.7	2.0	1.2
2.08	3.3	37.8	12	1.27	2.08	4.3	16.4	3.8	1.1
2.03	3.4	43.1	13	1.23	2.10	4.4	8.6	2.0	1.1
2.11	3.5	28.0	8.0	1.2	1.98	4.4	31.5	7.2	0.97
2.05	3.5	38.5	11	1.2	2.10	4.5	15.3	3.4	1.0
2.17	3.6	11.5	3.2	1.3	2.02	4.6	19.8	4.3	0.97
2.16	3.6	22.1	6.1	1.2	1.97	4.6	19.8	4.3	0.97
2.16	3.7	7.6	2.1	1.3	2.03	4.8	12.4	2.6	0.99
2.19	3.7	9.2	2.5	1.3	2.03	4.8	19.4	4.0	0.94
2.12	3.7	26.1	7.1	1.2	1.93	4.8	40.4	8.4	0.88
2.12	3.7	28.8	7.8	1.2	2.06	4.9	18.4	3.8	0.93
2.12	3.8	8.6	2.3	1.3	2.06	4.9	18.9	3.9	0.92
2.07	3.9	37.2	9.5	1.1	1.99	5.1	12.0	2.4	0.95
2.06	3.9	44.3	11	1.1	2.00	5.2	11.4	2.2	0.94
2.12	4.0	9.7	2.4	1.2	2.00	5.2	22.2	4.3	0.86
2.18	4.0	11.6	2.9	1.2	1.90	5.3	40.8	7.7	0.80
2.02	4.0	41.3	10	1.1	2.00	5.4	18.2	3.4	0.85
2.15	4.1	12.7	3.1	1.1	1.95	5.5	8.5	1.6	0.96
2.13	4.1	13.4	3.3	1.1	1.96	5.5	18.4	3.4	0.84
2.04	4.1	16.9	4.1	1.1	1.97	5.5	23.6	4.3	0.81
2.00	4.1	40.2	9.8	1.0	1.94	6.2	14.0	2.3	0.79
2.06	4.2	16.5	3.9	1.1	1.93	6.4	17.6	2.8	0.74
2.02	4.2	20.2	4.8	1.1					

\* (SA/V) = (2/L) + (4/d), from the Table 1

5). Extended Data Table S5.

Table S5. Au-0D-NP's $\lambda_{QGD}$ , $\tilde{\nu}_{QGD}$ and $\lambda_{SPR}$			
d (nm)	$\lambda_{QGD} = d/6$ (nm)	$\tilde{\nu}_{QGD} = 6/d$ (nm <sup>-1</sup> )	$\lambda_{SPR}$ (nm)
10	1.67	0.60	517.5
15	2.5	0.40	520
20	3.33	0.30	524
30	5	0.20	526
40	6.67	0.15	530
50	8.33	0.12	535
60	10	0.10	540
80	13.33	0.075	553
100	16.67	0.060	572

## 6). Extended Data Table S6.

Table S6. Main-group atoms polarizability, electronegativity, 1 <sup>st</sup> IP, and $\tilde{\nu}_{GW}$											
Atom	Polarizability <sup>(3)</sup> (10 <sup>-24</sup> cm <sup>3</sup> )	EN <sup>(3)</sup>	1st IP <sup>(3)</sup> (eV)	d/6 <sup>(3),(11)</sup> (nm)	6/d (nm <sup>-1</sup> )	Atom	Polarizability <sup>(3)</sup> (10 <sup>-24</sup> cm <sup>3</sup> )	EN <sup>(3)</sup>	1st IP <sup>(3)</sup> (eV)	d/6 <sup>(3),(11)</sup> (nm)	6/d (nm <sup>-1</sup> )
H	0.667	2.2	13.598	0.0177	56.6	Ge	6.07	2.01	7.899	0.0417	24.0
He	0.205		24.587	0.0103	96.8	As	4.31	2.18	9.789	0.038	26.3
Li	24.3	0.98	5.391	0.0555	18.0	Se	3.72	2.55	9.752	0.0342	29.2
Be	5.6	1.57	9.322	0.0373	26.8	Br	3.05	2.96	11.814	0.0313	31.9
B	3.03	2.04	8.298	0.029	34.5	Kr	2.48		14.0	0.0293	34.1
C	1.76	2.55	11.26	0.0223	44.8	Rb	47.3	0.82	4.177	0.0885	11.3
N	1.1	3.04	14.534	0.0187	53.6	Sr	27.6	0.95	5.695	0.073	13.7
O	0.802	3.44	13.618	0.016	62.5	In	10.2	1.78	5.786	0.0518	19.3
F	0.557	3.98	17.423	0.01	71.5	Sn	7.7	1.96	7.344	0.0483	20.7
Ne	0.39		21.565	0.0127	78.9	Sb	6.6	2.05	8.608	0.0442	22.6
Na	24.08	0.93	5.139	0.0633	15.8	Te	5.5	2.1	9.01	0.041	24.4
Mg	10.6	1.31	7.646	0.0483	20.7	I	5.35	2.66	10.451	0.0342	29.2
Al	6.8	1.61	5.986	0.0393	25.4	Xe	2.6	2.6	12.13	0.036	27.8
Si	5.38	1.90	8.152	0.0369	27.1	Cs	59.6	0.79	3.894	0.099	10.1
P	3.63	2.19	10.487	0.0327	30.6	Ba	39.7	0.89	5.212	0.084	11.9
S	2.9	2.58	10.36	0.0293	34.1	Tl	7.6	1.8	6.108	0.0623	15.8
Cl	2.18	3.16	12.968	0.0263	38.0	Pb	6.8	1.8	7.417	0.0513	19.5
Ar	1.62		15.76	0.0236	42.3	Bi	7.4	1.9	7.286	0.0476	21.0
K	43.3	0.82	4.341	0.0806	12.4	Po	6.8	2.0	8.417	0.045	22.2
Ca	22.8	1.00	6.113	0.0645	15.5	At	6.0	2.2		0.0424	23.6
Ga	8.12	1.81	5.999	0.0452	22.1	Rn	2.2		10.749	0.040	25.0

Note: The superscripts (3) and (11) represent the References #3 and #11.

## 7). Extended Data Table S7.

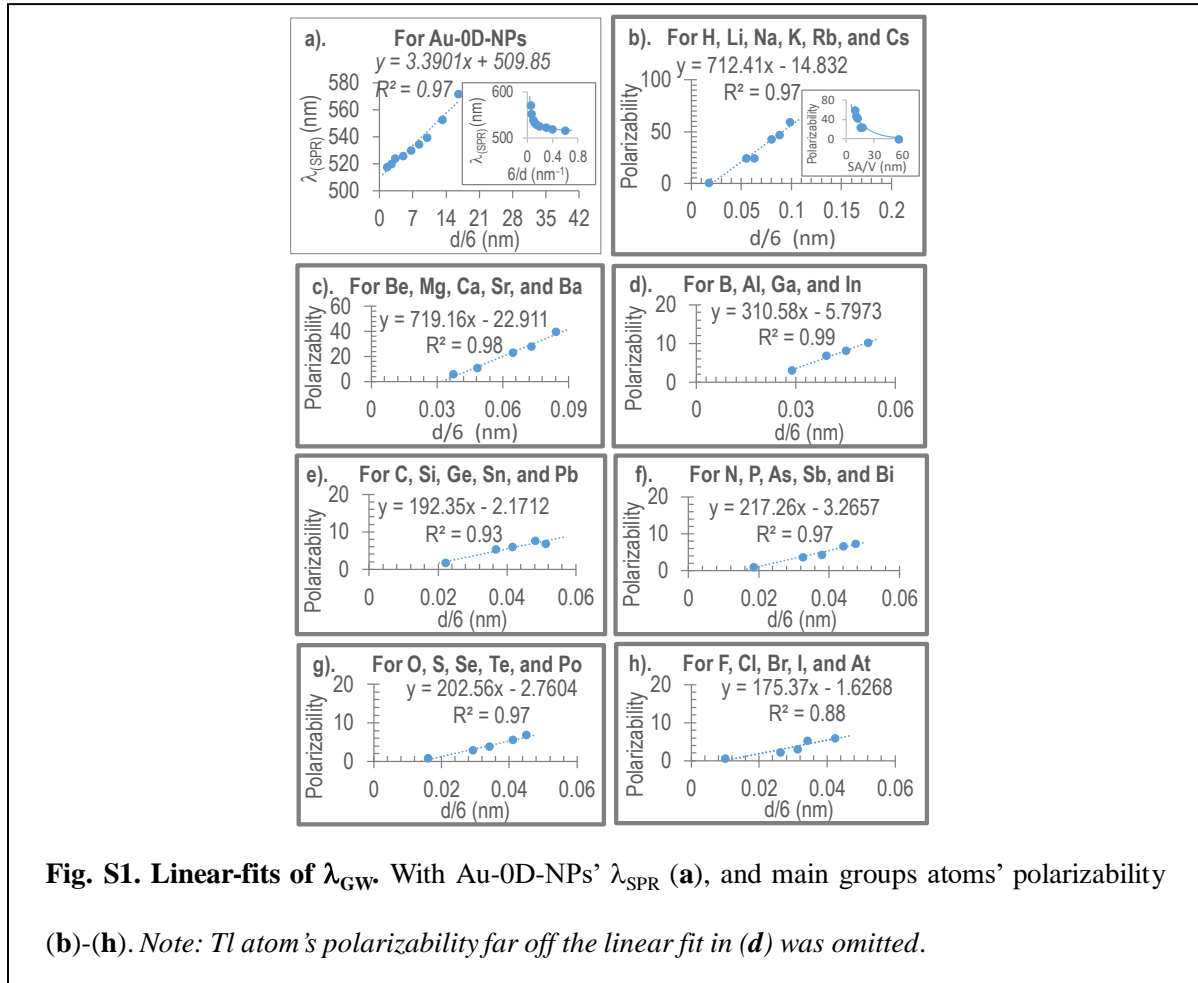
<b>Table S7. High-valent monoatomic cations <math>\tilde{\nu}_{GW}</math> and ionization potentials</b>							
<b>Cation</b>	<b>d/2 (nm)</b>	<b>6/d (nm<sup>-1</sup>)</b>	<b>IP (eV)</b>	<b>Cation</b>	<b>d/2 (nm)</b>	<b>6/d (nm<sup>-1</sup>)</b>	<b>IP (eV)</b>
V (II)	0.079	37.97	29.311	Mn (II)	0.083	36.14	33.668
V (III)	0.064	46.88	46.71	Mn (III)	0.058	51.72	51.2
V (IV)	0.058	51.72	65.28	Mn (IV)	0.053	56.6	72.4
V (V)	0.054	55.56	128.13	Mn (V)	0.033	90.91	95.6
				Mn (VI)	0.026	115.38	119.203
Cr (II)	0.073	41.1	30.96	Mn (VII)	0.025	120	194.5
Cr (III)	0.062	48.39	49.16				
Cr (IV)	0.055	54.55	90.635	Mo (III)	0.069	43.48	46.4
Cr (VI)	0.044	68.18	160.18	Mo (IV)	0.065	46.15	54.49
				Mo (V)	0.061	49.18	68.83
				Mo (VI)	0.059	50.85	125.67

8). Extended Data Table S8.

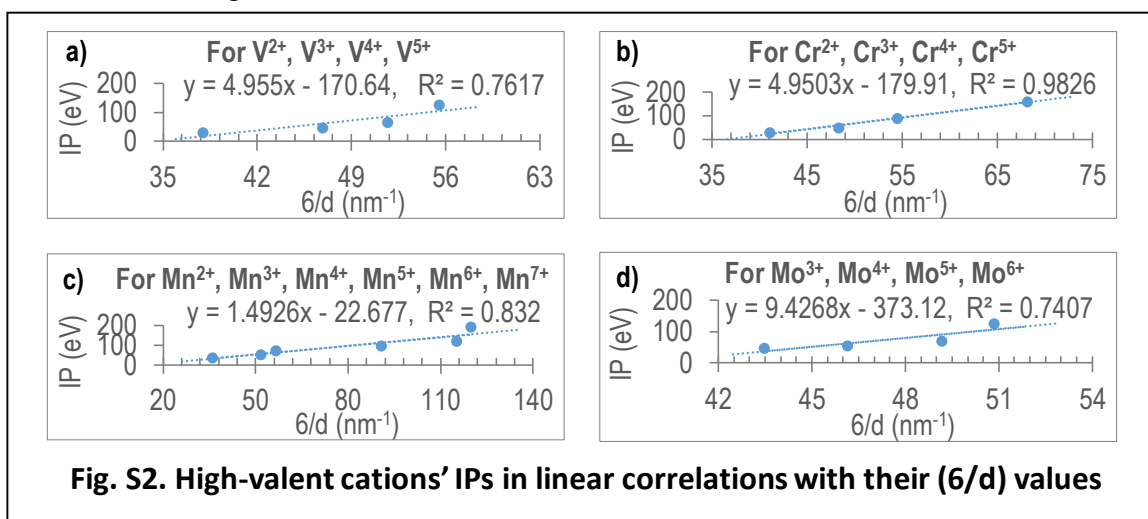
Table S8. PbSe 0D-NP	
$E_g$ (eV)	$6/d$ (nm <sup>-1</sup> )
0.833	1.18
0.967	1.40
1.077	1.58
1.243	1.88
1.656	2.61

## II. Extended Data Figures:

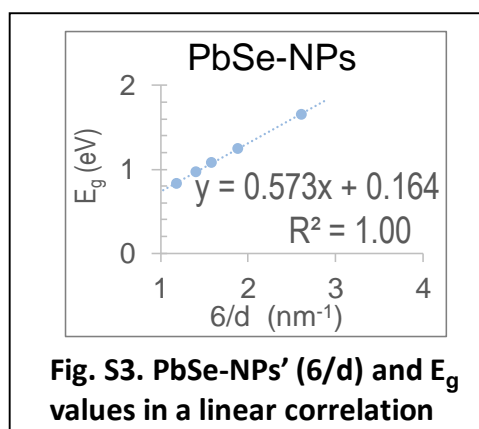
1). Extended Data Fig. S1.



2). Extended Data Fig. S2.



3). Extended Data Fig. S3.



4). Extended Data Fig. S4.

