

Title: **The geometrowave potential quantified and unified chemical properties**

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To date, size-dependent properties for atoms, ions, clusters, molecules, nanoparticles (or NPs) haven't been quantitatively predicted, differentiated, and unified, leaving many questions long-unanswered in chemistry. This work has introduced a geometrowave-number ($\tilde{\nu}_{GW}$) and GW-potential (μ_{GW}) to quantitatively predict, compare, and unify these particles' size-dependent properties. Such geometry-quantized chemical properties quantify the energy (or spontaneity) in self-assemble bonding, macromolecules' folding–unfolding, surface defects' reactivity, ions' GW-electronegativity, and NPs' redox change.

If predicting 64 Au-NPs (each 2-nm large) spontaneous self-assembly to an 8-nm NP, directly (*Route-A*) or stepwise (*Route B* + *Route C*) (**Fig. 1a**), each route's Gibbs free energy change¹ $\Delta G < 0$, supposedly. In chemical thermodynamics, however, NP formation's enthalpy (ΔH_f), entropy (ΔS_f), and ΔG_f ($\approx \Delta H_f - T\Delta S_f$) are unquantified or undefined, leaving self-assemblies²⁻⁷ never predicted and compared quantitatively.

To tackle many such problems in the thermodynamics- and quantum mechanics

(QM)-based general chemistry, let's quantize the zero-dimensional (0D), 1D-, 2D- and 3D-particles' Surface Area-to-Volume (SA/V) ratio (see the **Extended Data Table S1**) into a geometrowave-number ($\tilde{\nu}_{GW}$) with a unit of (length^{-1}). Thus, at $T = 298.15$ ($^{\circ}\text{K}$) and 1 (atm), the GW-potential $\mu_{f\text{GW}}^{\circ} = hc \cdot \tilde{\nu}_{GW}$, where the c = speed of light, h = Planck constant, and $hc \approx 1.24$ ($\text{keV} \cdot \text{nm}$). Therefore,

$$\begin{aligned}\Delta\mu_{f\text{GW(Route-A)}}^{\circ} &= \mu_{f\text{GW(8nm-NP)}}^{\circ} - 64\mu_{f\text{GW(2nm-NPs)}}^{\circ} \\ &= \{6/8 - 64(6/2)\}hc = -237.2 \text{ (keV)},\end{aligned}$$

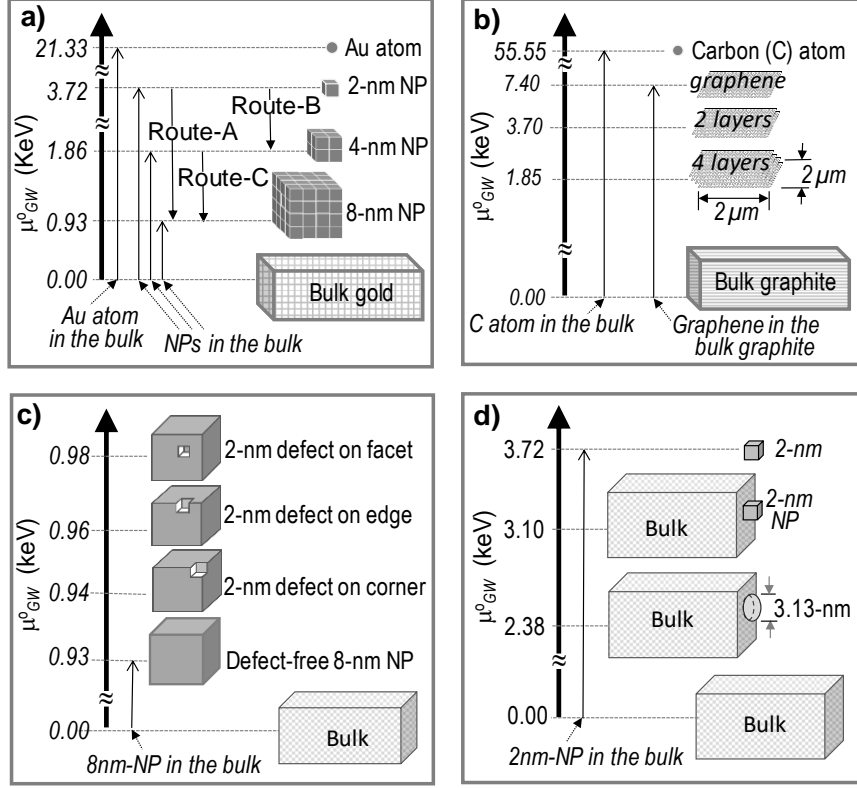


Fig. 1. The μ°_{GW} values. For the Au-NPs self-assembly (a), the graphene-layers (b), a 2-nm surface-defects on an 8-nm NP (c), and a 2-nm NP's adsorption and sintering on a large surface (d).

$$\Delta\mu^\circ_{fGW(\text{Route-B})} = 8\mu^\circ_{fGW(4\text{nm-NPs})} - 64\mu^\circ_{fGW(2\text{nm-NPs})}$$

$$= \{8(6/4) - 64(6/2)\}\hbar c = -223.2 \text{ (keV)},$$

$$\Delta\mu^\circ_{fGW(\text{Route-C})} = \mu^\circ_{fGW(8\text{nm-NP})} - 8\mu^\circ_{fGW(4\text{nm-NPs})}$$

$$= \{6/8 - 8(6/4)\}\hbar c = -14.0 \text{ (keV)}, \text{ and}$$

$$\Delta\mu^\circ_{fGW(\text{Route-A})} = \Delta\mu^\circ_{fGW(\text{Route-B})} + \Delta\mu^\circ_{fGW(\text{Route-C})},$$

confirming the $\Delta\mu^\circ_{fGW}$ as a state function.

Accordingly, a NP's μ°_{fGW} reduction in the hierarchical self-assembly bonding

(see the **Extended Data Table S2a**) is quantifiable:

$$\Delta\mu^\circ_{fGW(2\text{nm-NP in } 8\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-A})}/64 = -3.71$$

$$\text{(keV)} = -(99.73\% \cdot \mu^\circ_{fGW(2\text{nm-NP})}),$$

$$\Delta\mu^\circ_{fGW(2\text{nm-NP in } 4\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-B})}/64 = -3.49$$

$$\text{(keV)} = -(96.16\% \cdot \mu^\circ_{fGW(2\text{nm-NP})}),$$

$$\Delta\Delta\mu^\circ_{fGW(4\text{nm-NP in } 8\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-C})}/8 = -1.75$$

$$\text{(keV)} = -(94.09\% \cdot \mu^\circ_{fGW(4\text{nm-NP})}).$$

These equations indicate smaller NPs' inter-bonding stronger than larger NPs', matching a stronger bonding between smaller atoms. Every NP's $\mu_{f\text{GW}}^0$ loses nearly 100% in the bulk, since the $\tilde{V}_{\text{GW}(\text{bulk})}^0 = 0$ i.e. $\mu_{f\text{GW}(\text{bulk})}^0 = 0$. This hierarchical bonding, driven by minimizing smaller particles higher $\mu_{f\text{GW}}^0$ and generalizable to all self-assemblies²⁻⁷, can complement with the electron-centered Chemical Bonding⁸ Theory.

If assuming the $\Delta H_{f\text{GW}}^0 \ll \Delta \mu_{f\text{GW}}^0$ in the self-assembly, then the $\Delta S_{f\text{GW}(\text{environment})}^0 = -\Delta H_{f\text{GW}}^0/T \approx 0$, and $\Delta S_{f\text{GW}}^0 \approx -\Delta \mu_{f\text{GW}}^0/T > 0$. This helps predict quantitatively the $S_{f\text{GW}}^0$ to complement with Boltzmann entropy-based thermodynamics.

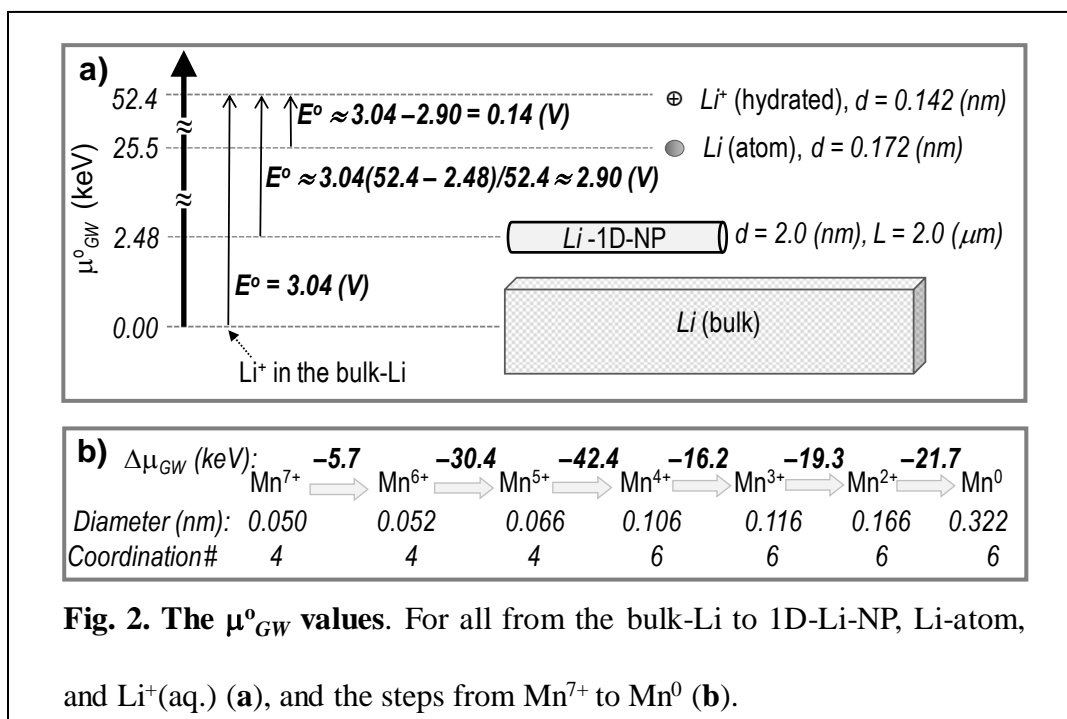
If folding a 150-nm long 1D-polyethylene (PE) to an 8-nm NP (or backward unfolding), since the $d_{(\text{ethylene})} \approx 0.390 \text{ (nm)}$ ⁹, the $\Delta \mu_{f\text{GW}(\text{Folding})}^0 = \mu_{f\text{GW}(\text{0D-PE-NP})}^0 - \mu_{f\text{GW}(\text{1D-PE-oligomer})}^0 \approx (6/8)hc - (4/0.390)hc = -11.78 \text{ (keV)} = -$

$\Delta \mu_{f\text{GW}(\text{Unfolding})}^0$. This can help generalize a thinner 1D-NP's greater $\mu_{f\text{GW}}^0$ for quantifying macromolecules inter-bonding (see the **Extended Data Tables S1 & S2a**).

For a mole of 8-nm NPs at $T = 298$ ($^\circ\text{K}$), the $\mu_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0 = 0.93 \text{ (keV/NP)} \times (6.023 \times 10^{23}) \text{ (NP/mole)} \times (1.60 \times 10^{-19}) \text{ (kJ/keV)} \approx 8.96 \times 10^4 \text{ (kJ/mole)}$. Accordingly, the $S_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0 = -\mu_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0/298 \approx -3.01 \times 10^5 \text{ (J/K}\cdot\text{mole)}$.

Given the $\Delta \mu_{f\text{GW}(\text{bulk graphite})}^0 = 0$ and $d_{(\text{C-atom})} \approx 0.134 \text{ (nm)}$ ¹⁰, the $\mu_{f\text{GW}}^0$ (see the **Extended Data Table S2b**) helps characterize large graphenes of different layers ($\sim 0.335 \text{ nm/layer}$) (**Fig. 1b**). The **Fig. 1b** can help quantify all thinner 2D-materials' higher $\mu_{f\text{GW}}^0$ generally.

On an 8nm-NP, the $\mu_{f\text{GW}}^0$ values of 2.0 nm-large surface vacancy defects (see the **Extended Data Table S2c**) are facet-defect's $>$ edge-defect's $>$ corner-defect's (**Fig. 1c**).

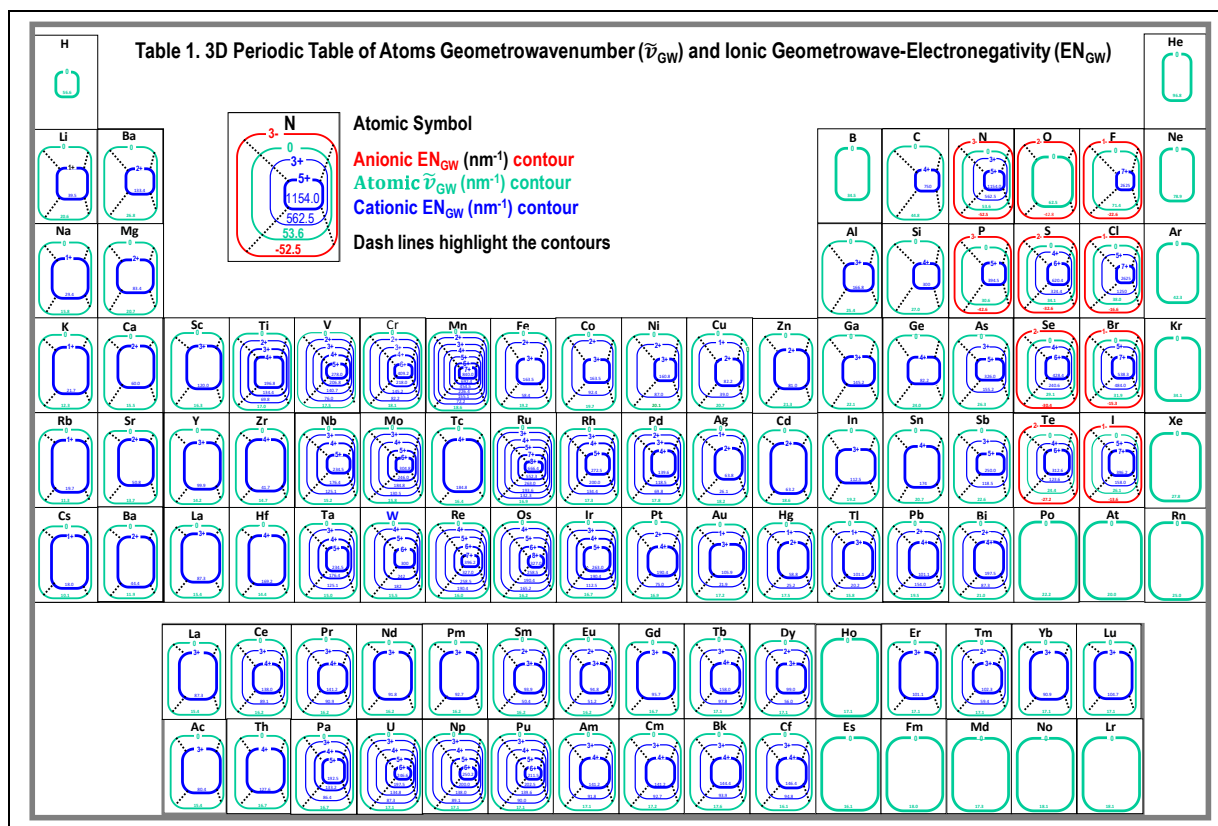


This helps generalize smaller defects' higher reactivity in the same order, to help study e.g. zeolites pores, proteins pockets and channels, and semiconductor surface vacancy defects.

On a bulk flat surface, the 2.0 nm-sized NP's spontaneous adsorption and "sintering" (see the **Extended Data Table S2d**) are each quantitatively characterizable (**Fig. 1d**). This can help quantitatively predict the μ°_{fQGD} in Surface Chemistry and Catalytic Chemistry, generally.

In Li-ion batteries¹¹⁻¹³, the electrochemically hard-to-measuring¹⁴

reduction potential from a $\text{Li}^+(\text{aq.})$ ¹⁵ to a 2- μm -long, 2-nm-thick Li-1D-NP electrode (**Fig. 2a**) is estimable (see the **Extended Data Table S2e**), i.e. $E^\circ_{(\text{cation-to-NP})} = E^\circ_{(\text{cation-to-bulk})} \cdot (\mu^\circ_{\text{fGW}(\text{cation})} - \mu^\circ_{\text{fGW}(\text{NP})}) / \mu^\circ_{\text{fGW}(\text{cation})} \approx -2.90$ (V). This can help quantify the $\Delta\mu^\circ_{\text{fGW}}$ (**Fig. 2b**) between NPs, atoms, and ions (see the **Extended Data Tables S2f, S3 & S4**) for expanding the electrochemistry, redox chemistry, and Lewis acid-base chemistry, using ions' GW-electronegativity ($\text{EN}_{\text{GW}} = (6/d) \times \pm(\text{ion's charge})$) (**Table 1**). Thus, the $\text{EN}_{\text{GW}} = -(\text{GW-electropositivity, or } \text{EP}_{\text{GW}})$,



for quantifying all ions' Lewis acidity (or basicity) in their compounding effectively using their EN_{GW} values.

The **Extended Data Table S1** supports a new nomenclature, " $\tilde{\nu}_{GW}$ -(point-group)-composition", for characterizing NPs-bonded countless compounds. For example, an 1.5-nm PbS-0D-NP can be thus-labeled as (6/1.5)-(R₃)-PbS, a 10-nm 0D-ZnSe-NP as (6/10)-(R₃)-ZnSe, their 1:1 compound as (6/1.5)-(R₃)-PbS•(6/10)-(R₃)-ZnSe, the 1.5-nm PbS-0D-NPs' linear

100mer as 1D-{(6/1.5)-(D_{∞d})-PbS}₁₀₀, and a 2-nm 0D-ZnO-NP's compound with a kinesin as (6/3)-(R₃)-ZnO-NP•kinesin, respectively.

In conclusion, the thermodynamics- and QM-complemented $\mu_f^o_{GW}$ has enabled consistently unifying and quantitatively predicting and comparing the particles' $\mu_f^o_{GW}$ -quantized properties including their hierarchical self-assembly bonding, redox activity, folding–unfolding, acidity and/or basicity, surface defects reactivity, etc.

Atoms' and monoatomic ions' EN_{GW} values could help develop new basics for (see in **Extended Data Table S3**), potentially overhauling modern chemistry¹⁶, which generalizable to the particles and oligomers, should be discussed separately.^{17,18}

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EXTENDED DATA.

I. Extended Data Tables S1–S4.





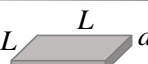



II. References.

Title: **The geometrowave potential quantified and unified chemical properties**

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I. Extended Data Tables.

1). Extended Data¹ TableS1:

Table S1. Simple-Shape Particles' $\tilde{\nu}_{GW}$ and Point Group (Symmetry)					
	Shape	Surface-Area (SA)	Volume (V)	$\tilde{\nu}_{GW}(= SA/V)$	Point Group
0D	 d	πd^2	$\pi d^3/6$	$(6/d)^*$	R_3
1D	 L d	$4dL + 2d^2$	$d^2 L$	$(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$	D_{4d}
	 L d	$\pi d^2/2 + \pi dL$	$\pi d^2 L/4$	$(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$	$D_{\infty d}$
2D	 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	$2(dL + dL + L^2)$	dL^2	$2/d + 2/L + 2/L;$ or $2/d$ if $d \ll L$	D_{4d}
3D	 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:

Table S2. Calculations of the μ_{GW}^0

a) $\mu_{GW}^0(\text{Au-atom}) = (17.2)hc = 21.33 \text{ (keV)},$
 $\mu_{GW}^0(2\text{nm-AuNP}) = (6/2)hc = 3.72 \text{ (keV)},$
 $\mu_{GW}^0(4\text{nm-AuNP}) = (6/4)hc = 1.86 \text{ (keV)},$
 $\mu_{GW}^0(8\text{nm-AuNP}) = (6/8)hc = 0.93 \text{ (keV)}.$

b) $\mu_{GW}^0(\text{C-atom}) = (44.8)hc = 55.55 \text{ (keV)},$
 $\mu_{GW}^0(1\text{-layer graphene}) = hc\{2/(1 \times 0.335)\} = 7.40,$
 $\mu_{GW}^0(2\text{-layer graphene}) = hc\{2/(2 \times 0.335)\} = 3.70 \text{ (keV)},$
 $\mu_{GW}^0(4\text{-layer graphene}) = hc\{2/(4 \times 0.335)\} = 1.85 \text{ (keV)}.$

c) $\mu_{GW}^0(\text{facet-defect}) = hc\{(SA/V)_{(2\text{-nm defect on } 8\text{-nm NP})}\} = hc\{(4 \times 2^2 + 6 \times 8^2)/(8^3 - 2^3)\} = hc\{(4 \times 2^2 + 384)/504\} = 0.98 \text{ (keV)},$
 $\mu_{GW}^0(\text{edge-defect}) = hc\{(2 \times 2^2 + 384)/504\} = 0.96 \text{ (keV)},$
 $\mu_{GW}^0(\text{corner-defect}) = hc\{384/504 - 17.2\} = 0.94 \text{ (keV)}.$

d) $\mu_{GW}^0(2\text{nm-NP-on-large flat surface}) = hc\{(5 \times 2^2)/8\} = 3.10 \text{ (keV)},$
 $\mu_{GW}^0(\text{hemisphere-on-large flat surface}) = hc\{(\pi d^2)/(\pi d^3/6)\} \approx hc(6/d) = hc(6/3.13) = 2.38 \text{ (keV)}.$

e) $\mu_{GW}^0(\text{Li (I) hydrated cation}) = hc(SA/V)_{\text{hydrated-Li-(I)-cation}} = hc(6/0.142) = 52.4 \text{ (keV)},$
 $\mu_{GW}^0(\text{Li atom}) = hc(SA/V)_{\text{Li-atom}} = hc(20.6) = 25.5 \text{ (keV)},$
 $\mu_{GW}^0(\text{Li-1D-NP}) \approx hc(4/d) = hc(4/2) = 2.48 \text{ (keV)}.$

f) $\mu_{GW}^0(\text{Mn(VII)}) = hc(6/0.050) = 148.8 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(VI)}) = hc(6/0.052) = 143.1 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(V)}) = hc(6/0.066) = 112.7 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(IV)}) = hc(6/0.106) = 70.3 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(III)}) = hc(6/0.116) = 64.1 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(II)}) = hc(6/0.166) = 44.8 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(0)}) = hc(6/0.322) = 23.1 \text{ (keV)}.$

3. Extended Data¹ Table S3:

Table S3. Periodicities of Atoms \tilde{V}_{GW}																		He 0.062 96.8							
H 0.106 56.6 2.20		<div><div>La 0.390 15.4 1.10</div><div>Atomic Symbol Atomic diameter* (unit: (nm)) \tilde{V}_{GW} (unit: nm⁻¹) Pauling's EN**</div></div>												B 0.174 34.5 2.04		C 0.134 44.8 2.55		N 0.112 53.6 3.04		O 0.096 62.5 3.44		F 0.084 71.4 3.98		Ne 0.076 78.9	
Li 0.234 20.6 0.98		Be 0.224 26.8 1.57		<div>*Atomic diameters data source: https://en.wikipedia.org/wiki/Atomic_radii_of_the_elements_(data_page) (Jan-8-2019).</div> <div>**Pauling's EN data source: Lide, D. R. <i>CRC Handbook of Chem. and Phys.</i> (CRC Press, Boca Raton, FL, 2000).</div>																					
Na 0.380 15.8 0.93		Mg 0.290 20.7 1.31		Sc 0.368 16.3 1.36	Ti 0.352 17.0 1.54	V 0.342 17.5 1.63	Cr 0.332 18.1 1.66	Mn 0.322 18.6 1.55	Fe 0.312 19.2 1.83	Co 0.304 19.7 1.88	Ni 0.298 20.1 1.91	Cu 0.290 20.7 1.90	Zn 0.282 21.3 1.65	Ga 0.272 22.1 1.81	Ge 0.250 24.0 2.01	As 0.228 26.3 2.18	Se 0.206 29.1 2.55	Br 0.188 31.9 2.96	Kr 0.176 34.1						
Rb 0.530 11.3 0.82		Sr 0.438 13.7 0.95		Y 0.424 14.2 1.22	Zr 0.412 14.7 1.33	Nb 0.396 15.2 1.6	Mo 0.380 15.8 2.16	Tc 0.366 16.4 2.10	Ru 0.356 16.9 2.2	Rh 0.346 17.3 2.28	Pd 0.338 17.8 2.20	Ag 0.330 18.2 1.93	Cd 0.322 18.6 1.69	In 0.312 19.2 1.78	Sn 0.290 20.7 1.96	Sb 0.266 22.6 2.05	Te 0.246 24.4 2.1	I 0.230 26.1 2.66	Xe 0.216 27.8 2.60						
Cs 0.596 10.1 0.79		Ba 0.506 11.9 0.89		La 0.390 15.4 1.10	Hf 0.416 14.4 1.3	Ta 0.400 15.0 1.5	W 0.386 15.5 1.7	Re 0.376 16.0 1.9	Os 0.370 16.2 2.2	Ir 0.360 16.7 2.2	Pt 0.354 17.5 2.2	Au 0.348 17.2 2.4	Hg 0.342 17.5 1.9	Tl 0.312 15.8 1.8	Pb 0.308 19.5 1.8	Bi 0.286 21.0 1.9	Po 0.270 22.2 2.0	At 0.300 20.0 2.2	Rn 0.240 25.0						
		La 0.390 15.4 1.10	Ce 0.370 16.2 1.12	Pr 0.370 16.2 1.13	Nd 0.370 16.2 1.1	Pm 0.370 16.2 1.17	Sm 0.370 16.2 1.17	Eu 0.370 16.2 1.20	Gd 0.360 16.7 1.20	Tb 0.350 17.1 1.20	Dy 0.350 17.1 1.22	Ho 0.350 17.1 1.23	Er 0.350 17.1 1.24	Tm 0.350 17.1 1.25	Yb 0.350 17.1 1.25	Lu 0.350 17.1 1.0									
		Ac 0.390 15.4 1.1	Th 0.360 16.7 1.3	Pa 0.360 16.7 1.5	U 0.350 17.1 1.7	Np 0.350 17.1 1.3	Pu 0.350 17.1 1.3	Am 0.350 17.1 1.3	Cm 0.348 17.2 1.7	Bk 0.340 17.6 1.6	Cf 0.372 16.1 1.6	Es 0.372 16.1 1.6	Fm 0.334 18.0 1.6	Md 0.346 17.3 1.7	No 0.332 18.1 1.7	Lr 0.322 18.1 1.7									

2,3

Table S4. Monoatomic ions' EN_{GW} values

ions	C.N.*	r (nm)	6/d (nm ⁻¹)	EN _{SW} (nm ⁻¹)*	ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{SW}	ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{SW}	ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{SW}
F ⁻	6	0.133	22.6	-22.6	BK ⁺⁴	6	0.083	36.1	144.4	Cu ⁺¹	2	0.046	65.2	65.2	Ir ⁺³	6	0.068	44.1	132.3
Cl ⁻	6	0.181	16.6	-16.6		8	0.093	32.3	129.2		4	0.060	50.0	50.0	Ir ⁺⁴	6	0.063	47.6	190.4
Br ⁻	6	0.196	15.3	-15.3	Br ⁺⁵	3	0.031	96.8	484		6	0.077	39.0	39.0	Ir ⁺⁵	6	0.057	52.6	263
I ⁻	6	0.220	13.6	-13.6	Br ⁺⁷	4	0.025	120	840	Cu ⁺²	4	0.057	52.6	105.2	K ⁺¹	4	0.137	21.9	21.9
OH ⁻	4	0.135	22.2	-22.2		6	0.039	76.9	538.3		6	0.073	41.1	82.2		6	0.138	21.7	21.7
	6	0.137	21.9	-21.9	C ⁺⁴	4	0.015	200	800	Dy ⁺²	6	0.107	28.0	56.0		8	0.151	19.9	19.9
O ⁻²	2	0.121	24.8	-49.6		6	0.016	187.5	750		8	0.119	25.2	50.4		12	0.164	18.3	18.3
	6	0.140	21.4	-42.8	Ca ⁺²	6	0.100	30.0	60.0	Dy ⁺³	6	0.091	33.0	99.0	La ⁺³	6	0.103	29.1	87.3
	8	0.142	21.1	-42.2		8	0.112	26.8	53.6		8	0.103	29.1	87.3		8	0.116	25.9	77.7
S ⁻²	6	0.184	16.3	-32.6		10	0.123	24.4	48.8	Er ⁺³	6	0.089	33.7	101.1		10	0.127	23.6	708
Se ⁻²	6	0.198	15.2	-30.4		12	0.134	22.4	44.8		8	0.100	30.0	90.0		12	0.136	22.1	66.3
Te ⁻²	6	0.221	13.6	-27.2	Cd ⁺²	4	0.078	38.5	77.0	Eu ⁺²	6	0.117	25.6	51.2	Li ⁺¹	4	0.059	50.8	50.8
N ⁻³	6	0.171	17.5	-52.5		6	0.095	31.6	63.2		8	0.125	24.0	48.0		6	0.076	39.5	39.5
P ⁻³	6	0.212	14.2	-42.6		8	0.110	27.3	54.6		10	0.135	22.2	44.4		8	0.092	32.6	32.6
						12	0.131	22.9	45.8	Eu ⁺³	6	0.095	31.6	94.8	Lu ⁺³	6	0.086	34.9	104.7
Ac ⁺³	6	0.112	26.8	80.4	Ce ⁺³	6	0.101	29.7	89.1		8	0.107	21.1	63.3		8	0.097	30.9	92.7
Ag ⁺¹	4	0.100	30.0	30.0		8	0.114	26.3	78.9	F ⁺⁷	6	0.008	375	2625	Mg ⁺²	4	0.057	52.6	105.2
	6	0.115	26.1	26.1		10	0.125	24.0	72.0	Fe ⁺²	4	0.063	47.6	95.2		6	0.072	41.7	83.4
	8	0.128	23.4	23.4		12	0.134	22.4	67.2		6	0.061	49.2	58.4		8	0.089	33.7	67.4
Ag ⁺²	4	0.079	38.0	76.0	Ce ⁺⁴	6	0.087	34.5	138		8	0.092	32.6	65.2	Mn ⁺²	4	0.066	45.5	91.0
	6	0.094	31.9	63.8		8	0.097	30.9	123.6	Fe ⁺³	4	0.049	61.2	183.6		6	0.083	36.1	72.2
Al ⁺³	4	0.039	76.9	230.7		10	0.107	28.0	112		6	0.055	54.5	163.5		8	0.096	31.3	62.6
	5	0.048	62.5	187.5		12	0.114	26.3	105.2		8	0.078	38.5	115.5	Mn ⁺³	6	0.058	51.7	155.1
	6	0.054	55.6	166.8	Cf ⁺³	6	0.095	31.6	94.8	Ga ⁺³	4	0.047	63.8	191.4	Mn ⁺⁴	4	0.039	76.9	307.6
Am ⁺³	6	0.098	30.6	91.8	Cf ⁺⁴	6	0.082	36.6	146.4		6	0.062	48.4	145.2		6	0.053	56.6	226.4
	8	0.109	27.5	82.5		8	0.092	32.6	130.4	Gd ⁺³	6	0.094	31.9	95.7	Mn ⁺⁵	4	0.033	90.9	454.5
Am ⁺⁴	6	0.085	35.3	141.2	Cf ⁺⁵	3	0.012	250	1250		8	0.105	28.6	85.8	Mn ⁺⁶	4	0.026	115.4	692.4
	8	0.095	31.6	126.4	Cf ⁺⁷	4	0.008	375	2625	Ge ⁺²	6	0.073	41.1	82.2	Mn ⁺⁷	4	0.025	120	840
As ⁺³	6	0.058	51.7	155.2	Cm ⁺³	6	0.097	30.9	92.7	Ge ⁺⁴	4	0.039	76.9	307.6	Mo ⁺³	6	0.069	43.5	130.5
As ⁺⁵	4	0.034	88.2	441	Cm ⁺⁴	6	0.085	35.3	141.2		6	0.053	56.6	226.4	Mo ⁺⁴	6	0.065	46.2	184.8
	6	0.046	65.2	326		8	0.095	31.6	126.4	Hf ⁺⁴	4	0.058	51.7	206.8	Mo ⁺⁵	4	0.046	65.2	326
Au ⁺¹	6	0.137	21.9	21.9	Co ⁺²	4	0.056	53.6	107.2		6	0.071	42.3	169.2		6	0.061	49.2	246
Au ⁺³	4	0.064	46.9	140.7		6	0.065	46.2	92.4		8	0.083	36.1	144.4	Mo ⁺⁶	4	0.041	73.2	439.2
	6	0.085	35.3	105.9		8	0.090	33.3	66.6	Hg ⁺¹	6	0.119	25.2	25.2		6	0.059	50.8	304.8
Ba ⁺²	6	0.135	22.2	44.4	Co ⁺³	6	0.055	54.5	163.5	Hg ⁺²	2	0.069	43.5	87.0		7	0.073	41.1	246.6
	8	0.142	21.1	42.2	Cr ⁺²	6	0.073	41.1	82.2		4	0.096	31.3	62.6	Ni ⁺³	6	0.016	187.5	562.5
	12	0.161	18.6	37.2	Cr ⁺³	6	0.062	48.4	145.2		6	0.102	29.4	58.8	Ni ⁺⁵	6	0.013	230.8	1154
Be ⁺²	4	0.027	111.1	222.2	Cr ⁺⁴	4	0.041	73.2	292.8		8	0.114	26.3	52.6	Na ⁺¹	4	0.099	30.3	30.3
	6	0.045	66.7	133.4		6	0.055	54.5	218	I ⁺⁵	3	0.044	68.2	341		6	0.102	29.4	29.4
Bi ⁺³	5	0.096	31.3	93.9		6	0.026	115.4	692.4		6	0.095	31.6	158		8	0.118	25.4	25.4
	6	0.103	29.1	87.3	Cr ⁺⁶	4	0.044	68.2	409.2	I ⁺⁷	4	0.042	71.4	499.8		9	0.124	24.2	24.2
	8	0.117	25.6	76.8		6	0.046	68.2	409.2		6	0.053	56.6	396.2		12	0.13	23.1	23.1
Bi ⁺⁵	6	0.076	39.5	197.5	Cs ⁺¹	6	0.167	18.0	18.0		6	0.062	48.4	145.2	Nb ⁺³	6	0.072	41.7	125.1
Bk ⁺³	6	0.096	31.3	93.9		8	0.174	17.2	17.2	In ⁺³	4	0.062	48.4	145.2		8	0.079	38.0	114
						10	0.181	16.6	16.6		6	0.080	37.5	112.5					
						12	0.188	16.0	16.0										

*CN: Coordination Number, and CN = 6 for most cases in the **Table 1**

****EN_{GW} unit: (nm⁻¹)**

4). Extended Data Table S4 (continued):

Ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{GW}	Ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{GW}	Ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{GW}	Ions	C.N.	r (nm)	6/d (nm ⁻¹)	EN _{GW}
Nb ⁴⁺	6	0.068	44.1	177.6	Pr ⁴⁺	6	0.085	35.3	141.2	Sm ²⁺	6	0.119	25.2	50.4	Tm ²⁺	6	0.101	29.7	59.4
Nb ⁵⁺	4	0.048	62.5	312.5		8	0.096	31.3	125.2		8	0.127	23.6	47.2		7	0.109	27.5	55.0
	6	0.064	46.9	234.5	Pt ²⁺	4	0.060	50.0	100	Sm ³⁺	6	0.096	31.3	93.9	Tm ³⁺	6	0.088	34.1	102.3
	8	0.074	40.5	202.5		6	0.080	37.5	75.0		8	0.108	27.8	83.4		8	0.099	30.3	90.9
Nd ³⁺	6	0.098	30.6	91.8	Pt ⁴⁺	6	0.063	47.6	190.4		12	0.124	24.2	72.6	U ³⁺	6	0.103	29.1	87.3
	8	0.112	26.8	80.4	Pu ³⁺	6	0.100	30.0	90.0	Sn ⁴⁺	4	0.055	54.5	218	U ⁴⁺	6	0.089	33.7	134.8
	9	0.116	25.9	77.7	Pu ⁴⁺	6	0.086	34.9	139.6		6	0.069	43.5	174		8	0.100	30.0	120
	12	0.127	23.6	70.8	Pu ⁵⁺	6	0.074	40.5	202.5		8	0.081	37.0	148		12	0.117	25.6	102.4
Ni ²⁺	4	0.049	61.2	122.4	Pu ⁶⁺	6	0.071	42.3	211.5	Sr ²⁺	6	0.118	25.4	50.8	U ⁵⁺	6	0.076	39.5	197.5
	6	0.069	43.5	87.0	Rb ¹⁺	6	0.152	19.7	19.7		8	0.126	23.8	47.6	U ⁶⁺	2	0.045	66.7	400.2
Ni ³⁺	6	0.056	53.6	160.8		8	0.161	18.6	18.6		10	0.136	22.1	44.2		4	0.052	57.7	346.2
Np ³⁺	6	0.101	29.7	89.1		10	0.166	18.1	18.1		12	0.144	20.8	41.6		6	0.073	41.1	246.6
Np ⁴⁺	6	0.087	34.5	138		12	0.172	17.4	17.4	Ta ³⁺	6	0.072	41.7	125.1		8	0.086	34.9	209.4
Np ⁵⁺	6	0.075	40.0	200	Re ⁴⁺	6	0.063	47.6	190.4	Ta ⁴⁺	6	0.068	44.1	176.4	V ²⁺	6	0.079	38.0	76.0
Np ⁶⁺	6	0.072	41.7	250.2	Re ⁵⁺	6	0.058	51.7	258.5	Ta ⁵⁺	6	0.064	46.9	234.5	V ³⁺	6	0.064	46.9	140.7
Os ⁴⁺	6	0.063	47.6	190.4	Re ⁶⁺	6	0.055	54.5	327	Tb ³⁺	6	0.092	32.6	97.8	V ⁴⁺	5	0.053	56.6	226.4
Os ⁵⁺	6	0.058	51.7	258.5	Re ⁷⁺	4	0.038	78.9	552.3		8	0.104	28.8	86.4		6	0.058	51.7	206.8
Os ⁶⁺	6	0.055	54.5	327		6	0.053	56.6	396.2	Tb ⁴⁺	6	0.076	39.5	158		8	0.072	41.7	166.8
Os ⁸⁺	6	0.039	76.9	615.2	Rh ³⁺	6	0.067	44.8	134.4		8	0.088	34.1	136.4	V ⁵⁺	4	0.036	83.3	416.5
P ⁵⁺	4	0.017	176.5	882.5	Rh ⁴⁺	6	0.060	50.0	200	Tc ⁴⁺	6	0.065	46.2	184.8		5	0.046	65.2	326
	6	0.038	78.9	394.5	Rh ⁵⁺	6	0.055	54.5	272.5	Te ⁴⁺	4	0.066	45.5	182		6	0.054	55.6	278
Pa ³⁺	6	0.104	28.8	86.4	Ru ³⁺	6	0.068	44.1	132.3		6	0.097	30.9	123.6	W ⁴⁺	6	0.066	45.5	182
Pa ⁴⁺	6	0.090	33.3	133.2	Ru ⁴⁺	6	0.062	48.4	193.6	Te ⁶⁺	4	0.043	69.8	418.8	W ⁵⁺	6	0.062	48.4	242
Pa ⁵⁺	6	0.078	38.5	192.5	Ru ⁵⁺	6	0.057	52.6	263		6	0.056	53.6	321.6	W ⁶⁺	4	0.042	71.4	428.4
Pb ²⁺	6	0.119	25.2	50.4	Ru ⁷⁺	4	0.038	78.9	552.3	Th ⁴⁺	6	0.094	31.9	127.6		5	0.051	58.8	352.8
	8	0.129	23.3	46.6	Ru ⁸⁺	4	0.036	83.3	670.4		8	0.105	28.6	114.4		6	0.060	50.0	300
	10	0.140	21.4	42.8	S ⁴⁺	6	0.037	81.1	324.4		10	0.113	26.5	106	Y ³⁺	6	0.090	33.3	99.9
	12	0.149	20.1	40.2	S ⁶⁺	4	0.012	250	1500		12	0.121	24.8	99.2		8	0.102	29.4	88.2
Pb ⁴⁺	4	0.065	46.2	184.8		6	0.029	103.4	620.4	Ti ²⁺	6	0.086	34.9	69.8		9	0.108	27.8	83.4
	6	0.078	38.5	154	Sb ³⁺	4	0.076	39.5	118.5	Ti ³⁺	6	0.067	44.8	134.4	Yb ²⁺	6	0.102	29.4	58.8
	8	0.094	31.9	127.6		6	0.076	39.5	118.5	Ti ⁴⁺	4	0.042	71.4	285.6		8	0.114	26.3	52.6
Pd ²⁺	4	0.064	46.9	93.8	Sb ⁵⁺	6	0.060	50.0	250		6	0.061	49.2	196.8	Yb ³⁺	8	0.099	30.3	90.9
	6	0.086	34.9	69.8	Sc ³⁺	6	0.075	40.0	120		8	0.074	40.5	162		9	0.104	28.8	86.4
Pd ³⁺	6	0.076	39.5	118.5		8	0.087	34.5	103.5	Th ¹⁺	6	0.150	20.0	20.2	Zn ²⁺	4	0.060	50.0	100
Pd ⁴⁺	6	0.062	48.4	193.6	Se ⁴⁺	6	0.050	60.0	240		8	0.159	18.9	18.9		6	0.074	40.5	81.0
Pm ³⁺	6	0.097	30.9	92.7	Se ⁶⁺	4	0.028	107.1	642.6		12	0.170	17.6	17.6		8	0.090	33.3	66.6
	8	0.109	27.5	82.5		6	0.042	71.4	428.4	Ti ³⁺	4	0.075	40.0	120	Zr ⁴⁺	4	0.059	50.8	203.2
Pr ³⁺	6	0.099	30.3	90.9	Si ⁴⁺	4	0.026	115.4	461.6		6	0.089	33.7	101.1		6	0.072	41.7	166.8
	8	0.113	26.5	79.5		6	0.040	75.0	300		8	0.098	30.6	91.8		8	0.084	35.7	142.8
																9	0.089	33.7	134.8

II. References:

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- ³ For the N³⁻ and P³⁻ radii: <https://www.chemguide.co.uk/atoms/properties/atradius.html>.