The geometrowave potential quantified and unified properties in general chemistry

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In the thermodynamics- and quantum mechanics (QM)-pillared general chemistry, many size-dependent properties of particles e.g. atoms, ions, molecules, clusters, and nanoparticles (NPs) haven't been quantitatively predicted and unified to date. This work has introduced a geometrowave to quantitatively predict and consistently unify these particles' geometry-quantized properties to complement the thermodynamics and QM. The properties include self-assembled NPs' inter-bonding strength, NPs self-assembly spontaneity, ions' acidity and/or basicity, reactivity of particles of all charges and geometries, macromolecules' folding and unfolding, and defects of all sizes and shapes at different surface-sites.

If predicting a spontaneous self-assembly from 64 of 2-nm Au-NPs to an 8-nm NP, either directly (*Route-A*) or stepwise (*Routes B + C*) (**Fig. 1a**), each route's Gibbs free energy change[1] $\Delta G < 0$, per the ΔG's definition. In thermodynamics, however, the NPs' formation enthalpy (ΔH_f), entropy (ΔS_f), and ΔG_f ($\approx \Delta H_f - T\Delta S_f$) are unquantified, leaving the self-assemblies[2-7] chemistry unquantifiable, incomparable, and unpredictable.

To tackle this thermodynamics problem, 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 geometro-wavenumber ($\tilde{\nu}_{GW}$) in the same unit of (length^{-1}). Thus, at T = 298.15 (^{o}K) and 1 (atm), the $\tilde{\nu}_{GW}$-based GW-potential $\mu_f{}^{o}{}_{GW}$ =

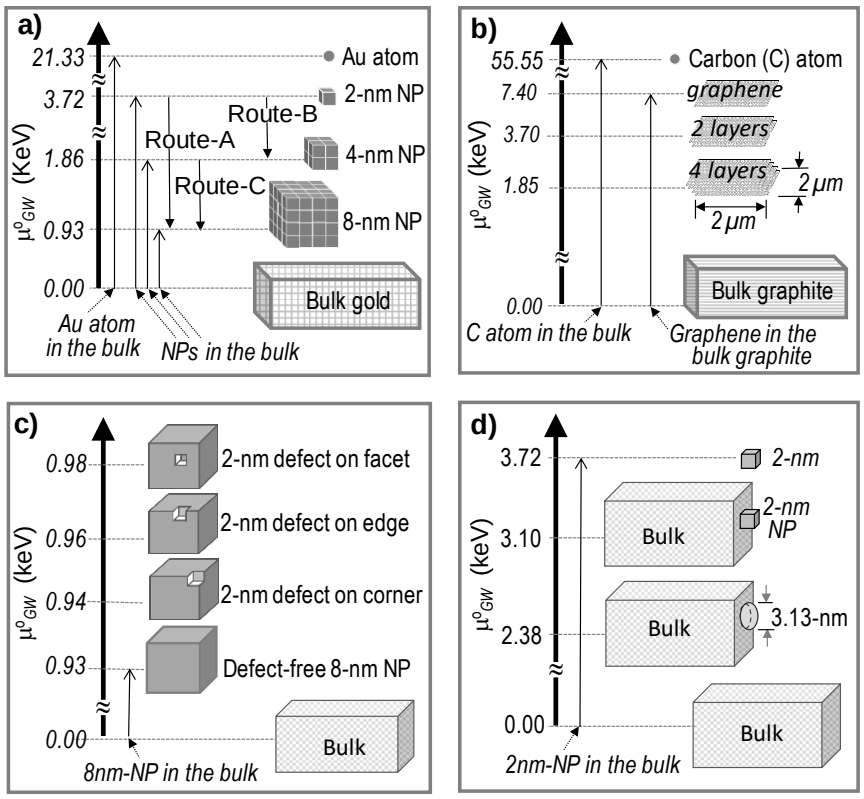


Fig. 1. The μ^{o}_{GW} values. For the Au-NPs self-assembly (**a**), the graphene-layers (**b**), a 2-nm surface-defects on an 8-nm NP (**c**), and a 2-nm NP's adsorption and sintering on a large surface (**d**).

$hc \cdot \tilde{\nu}_{GW}$, where the c = speed of light, h = Planck constant, and $hc \approx 1.24$ (keV·nm).

Accordingly, the

• $\Delta\mu_f{}^{o}{}_{GW(Route\text{-}A)} = \mu_f{}^{o}{}_{GW(8nm\text{-}NP)} - 64\mu_f{}^{o}{}_{GW(2nm\text{-}NPs)} = \{6/8 - 64(6/2)\}\hbar c = -237.2$ (keV),

• $\Delta\mu_f{}^{o}{}_{GW(Route\text{-}B)} = 8\mu_f{}^{o}{}_{GW(4nm\text{-}NPs)} - 64\mu_f{}^{o}{}_{GW(2nm\text{-}NPs)} = \{8(6/4) - 64(6/2)\}\hbar c = -223.2$ (keV),

• $\Delta\mu_f{}^{o}{}_{GW(Route\text{-}C)} = \mu_f{}^{o}{}_{GW(8nm\text{-}NP)} - 8\mu_f{}^{o}{}_{GW(4nm\text{-}NPs)} = \{6/8 - 8(6/4)\}\hbar c = -14.0$ (keV),

• $\Delta\mu_f{}^{o}{}_{GW(Route\text{-}A)} = \Delta\mu_f{}^{o}{}_{GW(Route\text{-}B)} + \Delta\mu_f{}^{o}{}_{GW(Route\text{-}C)}$, which proved that the $\Delta\mu_f{}^{o}{}_{GW}$ is a state function.

Therefore, every NP's $\mu_f{}^{o}{}_{GW}$ reduction in the hierarchical self-assembly bonding (see the **Extended Data Table S2a**) is likewise quantifiable:

• $\Delta\mu_f{}^{o}{}_{GW(2nm\text{-}NP\ in\ 8nm\text{-}NP)} = \Delta\mu_f{}^{o}{}_{GW(Route\text{-}A)}/64 = -3.71$ (keV) $= -(99.73\% \cdot \mu_f{}^{o}{}_{GW(2nm\text{-}NP)})$,

•$\Delta\mu_f{}^o{}_{GW(2nm\text{-}NP\ in\ 4nm\text{-}NP)} = \Delta\mu_f{}^o{}_{GW(Route\text{-}B)}/64 = -3.49$ (keV) = –(96.16%·$\mu_f{}^o{}_{GW(2nm\text{-}NP)}$),

•$\Delta\Delta\mu_f{}^o{}_{GW4nm\text{-}NP\ in\ 8nm\text{-}NP)} = \Delta\mu_f{}^o{}_{GW(Route\text{-}C)}/8 = -1.75$ (keV) = –(94.09%·$\mu_f{}^o{}_{GW(4nm\text{-}NP)}$).

These have concluded the larger NPs' inter-bonding weaker than smaller NPs', depending on NPs' geometry and regardless NPs' chemical composition, and every NP's $\mu_f{}^o{}_{GW}$-decrease near 100% in the bulk since $\tilde{\nu}^o{}_{GW(bulk)} = 0$ i.e. $\mu_f{}^o{}_{GW(bulk)} = 0$. This hierarchical bonding, driven by minimizing smaller particles higher $\mu_f{}^o{}_{GW}$ which is generalizable to all-scales' self-assemblies[2-7], can help expand the Chemical Bonding Theory[8].

Assuming $\Delta H_f{}^o{}_{GW} << \Delta\mu_f{}^o{}_{GW}$, then $\Delta S_f{}^o{}_{GW(environment)} = -\Delta H_f{}^o{}_{GW}/T \approx 0$, and $\Delta S_f{}^o{}_{GW} \approx -\Delta\mu_f{}^o{}_{GW}/T > 0$. This can help quantitatively predict the $S_f{}^o{}_{GW}$ and $\mu_f{}^o{}_{GW}$ (see the **Extended Data Table S1**) to expand the Boltzmann entropy-supported thermodynamics. For a mole of 8-nm NPs at T = 298 (°K),

•$\mu_{mf}{}^o{}_{GW(8nm\text{-}AuNP)} = 0.93$ (keV/NP) × (6.023×10^{23}) (NP/mole) × (1.60×10^{-19}) (kJ/keV) ≈ 8.96×10^4 (kJ/mole), and

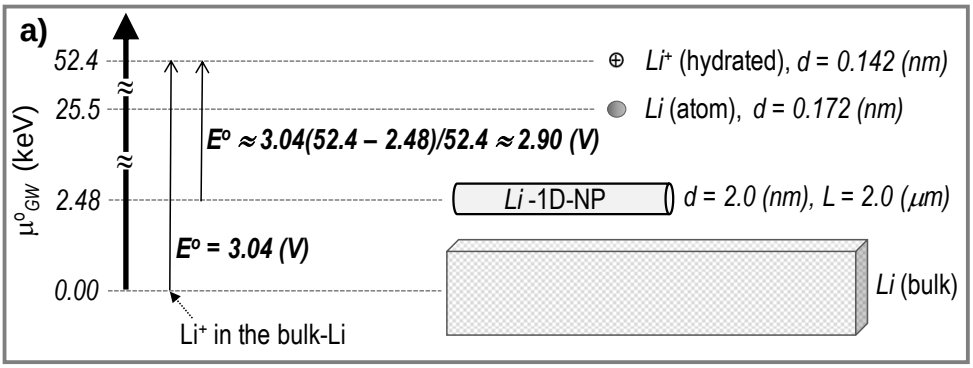
•$S_{mf}{}^o{}_{GW(8nm\text{-}AuNP)} = -\mu_{mf}{}^o{}_{GW(8nm\text{-}AuNP)}/298 \approx -3.01 \times 10^5$ (J/K·mole).

If folding a 150-nm long 1D-polyethylene (PE) to an 8-nm NP (or backward unfolding), given the $d_{(ethylene)} \approx 0.390$ (nm)[9], the

•$\Delta\mu_f{}^o{}_{GW(Folding)} = \mu_f{}^o{}_{GW(0D\text{-}PE\text{-}NP)} - \mu_f{}^o{}_{GW(1D\text{-}PE\text{-}oligomer)} \approx (6/8)hc - (4/0.390)hc = -11.78$ (keV) = $-\Delta\mu_f{}^o{}_{GW(Unfolding)}$.

This can help generalize a thinner 1D-NP's greater $\mu_f{}^o{}_{GW}$ (see the **Extended Data Table S1**) for quantifying macromolecules' chemical bonding, as exemplified in the **Extended Data Table S2a**.

Given the $\Delta\mu_f{}^o{}_{GW(bulk\ graphite)} = 0$ and $d_{(C\text{-}atom)} \approx 0.134$ (nm)[10], the $\mu_f{}^o{}_{GW}$ (see the **Extended Data Table S2b**) can help characterize large graphenes of different layers (~0.335 nm/layer) (**Fig. 1b**). The **Fig.**



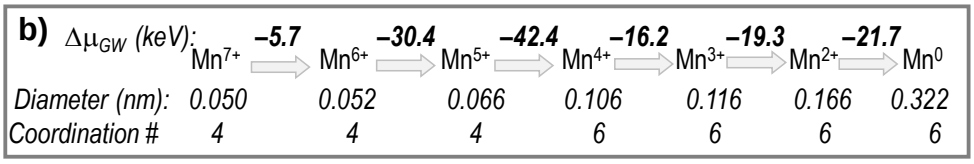


Fig. 2. The μ^{o}_{GW} values. Through the steps from the bulk-Li to 1D-Li-NP, Li-atom, and Li^{+}(aq.) (**a**), and that from Mn^{7+} to Mn^{0} (**b**).

1b can help quantify all thinner 2D-materials' higher $\mu_f{}^{o}_{GW}$ generally.

On an 8nm-NP, the $\mu_f{}^{o}_{GW}$ values of 2.0 nm-sized surface defects (see the **Extended Data Table S2c**) are facet-defect's > edge-defect's > corner-defect's (**Fig. 1c**). This can help generalize all smaller defects' higher reactivity in the same order, and in turn study quantitatively the zeolites pores, proteins pockets and channels, and semiconductor 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 $\mu_f{}^{o}_{QGD}$ in the Surface Chemistry and Catalytic Chemistry, generally.

In Li-ion batteries[11-13], the electrochemically hard-to-measuring[14] reduction potential from a Li^{+}(aq.)[15] to a 2-μm-long, 2-nm-thick Li-1D-NP electrode (**Fig. 2a**) is estimable (see the **Extended Data Table S2e**),

• $E^{o}_{(cation\text{-}to\text{-}NP)} = E^{o}_{(cation\text{-}to\text{-}bulk)} \cdot (\mu_f{}^{o}_{GW(cation)} - \mu_f{}^{o}_{GW(NP)})/\mu_f{}^{o}_{GW(cation)} \approx -2.90$ (V).

This can help quantify the $\Delta\mu_f{}^o{}_{GW}$ change (**Fig. 2b**) between NPs, atoms, and ions (see the **Extended Data Tables S2f&S3**) for expanding the electrochemistry, redox chemistry, and Lewis acid-base chemistry with ions' $\mu_f{}^o{}_{GW}$-quantified acidity and basicity e.g. (6/d)(ion-charges).

The **Extended Data Table S1** further supports a $\mu_f{}^o{}_{GW}$-generalized nomenclature, "$\tilde{\nu}_{GW}$-(point-group)-composition", for characterizing NP-compounds. For example, an 1.5-nm PbS-0D-NP can be thus-labeled as (6/1.5)-(R_3)-PbS, a 10-nm 0D-ZnSe-NP as (6/10)-(R_3)-ZnSe, their 1:1 compound as (6/1.5)-(R_3)-PbS•(6/10)-(R_3)-ZnSe, the 1.5-nm PbS-0D-NPs' linear 100mer as 1D-{(6/1.5)-($D_{\infty d}$)-PbS}$_{100}$, and a 2-nm 0D-ZnO-NP's compound with kinesin as (6/3)-(R_3)-ZnO-NP•kinesin.

In conclusion, the thermodynamics- and QM-complemented $\mu_f{}^o{}_{GW}$ enables us to consistently unify and quantitatively compare and predict the particles' GW-

Table 1. Periodicities of Atoms and Monoatomic Ions $\tilde{\nu}_{GW}$ Values

H 0.106 **56.6** *2.20*																	**He** 0.062 **96.8**
Li 0.234 **20.6** *0.98*	**Be** 0.224 **26.8** *1.57*											**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**
Na 0.380 **15.8** *0.93*	**Mg** 0.290 **20.7** *1.31*											**Al** 0.236 **25.4** *1.61*	**Si** 0.222 **27.0** *1.90*	**P** 0.196 **30.6** *2.19*	**S** 0.176 **34.1** *2.58*	**Cl** 0.158 **38.0** *3.16*	**Ar** 0.142 **42.3**
K 0.486 **12.3** *0.82*	**Ca** 0.388 **15.5** *1.00*	**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 **16.9** *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**	**Sm** 0.370 **16.2** *1.17*	**Eu** 0.370 **16.2**	**Gd** 0.360 **16.7** *1.20*	**Tb** 0.350 **17.1**	**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**	**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**	**Cm** 0.238 **25.2**	**Bk** 0.34 **17.6**	**Cf** 0.372 **16.1**	**Es** 0.372 **16.1**	**Fm** 0.334 **18.0**	**Md** 0.346 **17.3**	**No** 0.332 **18.1**	**Lr** 0.322 **18.1**	

La
0.308
19.5
1.10

Atomic Symbol
Atomic diameter* {unit: (nm)}
$\tilde{\nu}_{GW}$ **{unit: (nm^{-1})}**
*Pauling's EN***

*Atomic diameters data source:
https://en.wikipedia.org/wiki/Atomic_radii_of_the_elements_(data_page) (Jan-8-2019).

**Pauling's EN data source:
Lide, D. R. *CRC Handbook of Chem. and Phys.* (CRC Press, Boca Raton, FL, 2000).

quantized properties including their hierarchical self-assembly bonding, folding–unfolding, redox activity, acidity and basicity, surface defects reactivity, etc. Atoms' and monoatomic, monovalent ions' EN-complementary $\mu_f{}^{o}{}_{GW}$ (**Table 1**), generalizable to the particles and oligomers (**Extended Data Tables S1&S3**), can help develop new basics beyond the chemistry[16], which should be discussed separately.

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EXTENDED DATA.

I. **Extended Data Tables S1–S4.**

The eometrowave potential quantified and unified properties in general chemistry

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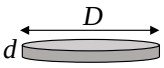
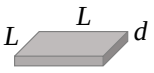
I. Extended Data Tables.

1). Extended Data Table S1**.**

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* $d << L$	D_{2d}
	 *L* *d*	$\pi d^2/2 + \pi dL$	$\pi d^2 L/4$	$(4/d + 2/L)$** or $(4/d)$** *if* $d << L$	$D_{\infty d}$
2D	 *D* *d*	$\pi D^2/2 + d\pi D$	$d\pi D^2/4$	$2/d + 4/D$; or $2/d$ *if* $d << D$	$D_{\infty d}$
	 *L* *L* *d*	$2(aL + aL + L^2)$	aL^2	$2/d + 2/L + 2/L$; or $2/d$ *if* $d << L$	D_{4d}
3D	 *d*	$6d^2$	d^3	$(6/d)$*	O_h
	 *d*	$2\times3^{1/2}d^2$	$2^{1/2}d^3/3$	$3\times6^{1/2}/d$	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^o_{GW}

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

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

c) $\mu^o_{GW(\text{facet-defect})} = hc\{(SA/V)_{(\text{2-nm defect on 8-nm NP})}\} = hc\{(4\times2^2 + 6\times8^2)/(8^3 - 2^3)\} = hc\{(4\times2^2 + 384)/504\} = 0.98$ (keV),
$\mu^o_{GW(\text{edge-defect})} = hc\{(2\times2^2 + 384)/504\} = 0.96$ (keV),
$\mu^o_{GW(\text{corner-defect})} = hc\{384/504 - 17.2\} = 0.94$ (keV).

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

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

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

3). Extended Data Table S3.

Table S3. Hydrated monoatomic ions' $\tilde{\nu}_{GW}$ values

ions	C.N.*	r (nm)	6/d (nm^{-1})	Basicity (nm^{-1})**
F^-	6	0.133	22.6	-22.6
Cl^-	6	0.181	16.6	-16.6
Br^-	6	0.196	15.3	-15.3
I^-	6	0.22	13.6	-13.6
OH^-	4	0.135	22.2	-22.2
	6	0.137	21.9	-21.9
O^{-2}	2	0.12	25.0	-50.0
	6	0.14	21.4	-42.8
	8	0.142	21.1	-42.2
S^{-2}	6	0.184	16.3	-32.6
Se^{-2}	6	0.198	15.2	-30.4
Te^{-2}	6	0.221	13.6	-27.2
				Acidity (nm^{-1})***
Ac^{+3}	6	0.112	26.8	80.4
Ag^{+1}	4	0.1	30.0	30.0
	6	0.115	26.8	26.8
	8	0.128	23.4	23.4
Ag^{+2}	4	0.079	38.0	76.0
	6	0.094	31.9	63.8
Al^{+3}	4	0.039	76.9	230.7
	5	0.048	62.5	187.5
	6	0.054	55.6	166.8
Am^{+3}	6	0.098	30.6	918
	8	0.109	27.5	82.5
Am^{+4}	6	0.085	35.3	141.2
	8	0.095	31.6	126.4
As^{+3}	6	0.058	51.7	155.1
As^{+5}	4	0.034	88.2	441
	6	0.046	65.2	326
Au^{+1}	6	0.137	21.9	21.9
Au^{+3}	4	0.064	46.9	140.7
	6	0.085	35.3	108.9
Ba^{+2}	6	0.135	22.2	44.4
	8	0.142	21.1	42.2
	12	0.161	18.6	37.2
Be^{+2}	4	0.027	111.1	222.2
	6	0.045	66.7	133.4
Bi^{+3}	5	0.096	31.3	93.9
	6	0.103	29.1	87.3
	8	0.117	25.6	76.8
Bi^{+5}	6	0.076	39.5	197.5
Br^{+5}	3	0.031	96.8	484

ions	C.N.	r (nm)	6/d (nm^{-1})	Acidity (nm^{-1})
Br^{+7}	4	0.025	120	840
	6	0.039	76.9	538.3
C^{+4}	4	0.015	200	800
	6	0.016	187.5	750
Ca^{+2}	6	0.1	30.0	60.0
	8	0.112	26.8	53.6
	10	0.123	24.4	48.8
	12	0.134	22.4	44.8
Cd^{+2}	4	0.078	38.5	77.0
	6	0.095	31.6	63.2
	8	0.11	27.3	54.6
	12	0.131	22.9	45.8
Ce^{+3}	6	0.101	29.7	89.1
	8	0.114	26.3	78.9
	10	0.125	24.0	72.0
	12	0.134	22.4	67.2
Ce^{+4}	6	0.087	34.5	138
	8	0.097	30.9	123.6
	10	0.107	28.0	112
	12	0.114	26.3	105.2
Cl^{+5}	3	0.095	31.6	158
Cl^{+7}	4	0.082	36.6	256.2
Co^{+2}	4	0.056	53.6	107.2
	6	0.065	46.2	92.4
	8	0.09	33.3	66.6
Co^{+3}	6	0.055	54.5	163.5
Cr^{+2}	6	0.073	41.1	82.2
Cr^{+3}	6	0.062	48.4	145.2
Cr^{+4}	4	0.041	73.2	292.8
	6	0.055	54.5	218
Cr^{+6}	4	0.026	115.4	692.4
	6	0.044	68.2	409.2
Cs^{+1}	6	0.167	18.0	18.0
	8	0.174	17.2	17.2
	10	0.181	16.6	16.6
	12	0.188	16.0	16.0
Cu^{+1}	2	0.046	65.2	65.2
	4	0.06	50.0	50.0
	6	0.077	39.0	39.0
Cu^{+2}	4	0.057	52.6	105.2
	6	0.073	41.1	82.2
F^{+7}	6	0.008	375.0	2625

ions	C.N.	r (nm)	6/d (nm^{-1})	Acidity (nr
Fe^{+2}	4	0.063	47.6	95.2
	6	0.061	49.2	58.4
	8	0.092	32.6	65.2
Fe^{+3}	4	0.049	61.2	183.6
	6	0.055	54.5	163.5
	8	0.078	38.5	115.5
Ga^{+3}	4	0.047	63.8	191.4
	6	0.062	48.4	145.2
Ge^{+2}	6	0.073	41.1	82.2
Ge^{+4}	4	0.039	76.9	307.6
	6	0.053	56.6	226.4
Hf^{+4}	4	0.058	51.7	206.8
	6	0.071	42.3	169.2
	8	0.083	36.1	144.4
Hg^{+1}	6	0.119	25.2	25.2
Hg^{+2}	2	0.069	43.5	87.0
	4	0.096	31.3	62.6
	6	0.102	29.4	58.8
	8	0.114	26.3	52.6
I^{+5}	3	0.044	68.2	341
	6	0.095	31.6	158
I^{+7}	4	0.042	71.4	499.8
	6	0.053	56.6	396.2
In^{+3}	4	0.062	48.4	145.2
	6	0.080	37.5	112.5
Ir^{+3}	6	0.068	44.1	132.3
Ir^{+4}	6	0.063	47.6	190.4
Ir^{+5}	6	0.057	52.6	263
K^{+1}	4	0.137	21.9	21.9
	6	0.138	21.7	21.7
	8	0.151	19.9	19.9
	12	0.164	18.3	18.3
La^{+3}	6	0.103	29.1	87.3
	8	0.116	25.9	77.7
	10	0.127	23.6	708
	12	0.136	22.1	66.3
Li^{+1}	4	0.059	50.8	50.8
	6	0.076	39.5	39.5
	8	0.092	32.6	32.6
Mg^{+2}	4	0.057	52.6	105.2
	6	0.072	41.7	83.4
	8	0.089	33.7	67.4

*C.N.: Coordination Number

**Basicity = (6/d) x (negative charges)

***Acidity = (6/d) x (positive charges)

3). Extended Data Table S3 (continued).

Table S3. Hydrated monoatomic ions' $\tilde{\nu}_{GW}$ values (continued)

ions	C.N.	r (nm)	6/d (nm^{-1})	Acidity (nm^{-1})	ions	C.N.	r (nm)	6/d (nm^{-1})	Acidity (nm^{-1})	ions	C.N.	r (nm)	6/d (nm^{-1})	Acidity (nm^{-1})
Mn^{+2}	4	0.066	45.5	91.0	Pb^{+4}	4	0.065	46.2	184.8	Sr^{+2}	6	0.118	25.4	50.8
	6	0.083	36.1	72.2		6	0.078	38.5	154.0		8	0.126	23.8	47.6
	8	0.096	31.3	62.6		8	0.094	31.9	127.6		10	0.136	22.1	44.2
Mn^{+3}	6	0.058	51.7	155.1	Pd^{+2}	4	0.064	46.9	93.8		12	0.144	20.8	41.6
Mn^{+4}	4	0.039	76.9	307.6		6	0.086	34.9	69.8	Ta^{+3}	6	0.072	41.7	125.1
	6	0.053	56.6	226.4	Pd^{+3}	6	0.076	39.5	118.5	Ta^{+4}	6	0.068	44.1	176.4
Mn^{+5}	4	0.033	90.9	454.5	Pd^{+4}	6	0.062	48.4	193.6	Ta^{+5}	6	0.064	46.9	234.5
Mn^{+6}	4	0.026	115.4	692.4	Pt^{+2}	4	0.06	50.0	100.0	Tc^{+4}	6	0.065	46.2	184.8
Mn^{+7}	4	0.025	120.0	840.0		6	0.08	37.5	75.0	Ti^{+2}	6	0.086	34.9	69.8
Mo^{+3}	6	0.069	43.5	130.5	Pt^{+4}	6	0.063	47.6	190.4	Ti^{+3}	6	0.067	44.8	134.4
Mo^{+4}	6	0.065	46.2	184.8	Rb^{+1}	6	0.152	19.7	19.7	Ti^{+4}	4	0.042	71.4	285.6
Mo^{+5}	4	0.046	65.2	326.0		8	0.161	18.6	18.6		6	0.061	49.2	196.8
	6	0.061	49.2	246.0		10	0.166	18.1	18.1		8	0.074	40.5	162
Mo^{+6}	4	0.041	73.2	439.2		12	0.172	17.4	17.4	Tl^{+1}	6	0.15	20.0	20.2
	6	0.059	50.8	304.8	Re^{+4}	6	0.063	47.6	190.4		8	0.159	18.9	18.9
	7	0.073	41.1	246.6	Re^{+5}	6	0.058	51.7	258.5		12	0.17	17.6	17.6
N^{+3}	6	0.016	187.5	562.5	Re^{+6}	6	0.055	54.5	327.0	Tl^{+3}	4	0.075	40.0	120
N^{+5}	6	0.013	230.8	1154.0	Re^{+7}	4	0.038	78.9	552.3		6	0.089	33.7	101.1
Na^{+1}	4	0.099	30.3	30.3		6	0.053	56.6	396.2		8	0.098	30.6	91.8
	6	0.102	29.4	29.4	Rh^{+3}	6	0.067	44.8	134.4	V^{+2}	6	0.079	38.0	76.0
	8	0.118	25.4	25.4	Rh^{+4}	6	0.06	50.0	200.0	V^{+3}	6	0.064	46.9	140.7
	9	0.124	24.2	24.2	Rh^{+5}	6	0.055	54.5	272.5	V^{+4}	5	0.053	56.6	226.4
	12	0.13	23.1	23.1	Ru^{+3}	6	0.068	44.1	132.3		6	0.058	51.7	206.8
Nb^{+3}	6	0.072	41.7	125.1	Ru^{+4}	6	0.062	48.4	193.6		8	0.072	41.7	166.8
	8	0.079	38.0	114.0	Ru^{+5}	6	0.057	52.6	263.0	V^{+5}	4	0.042	71.4	357
Nb^{+4}	6	0.068	44.1	177.6	Ru^{+7}	4	0.038	78.9	552.3		5	0.051	58.8	294
Nb^{+5}	4	0.048	62.5	312.5	Ru^{+8}	4	0.036	83.3	670.4		6	0.06	50.0	250
	6	0.064	46.9	234.5	S^{+4}	6	0.037	81.1	324.4	W^{+4}	6	0.066	45.5	182
	8	0.074	40.5	202.5	S^{+6}	4	0.012	250.0	1500.0	W^{+5}	6	0.062	48.4	242
Ni^{+2}	4	0.049	61.2	122.4		6	0.029	103.4	620.4	W^{+6}	4	0.042	71.4	428.4
	6	0.069	43.5	87.0	Sb^{+3}	4	0.076	39.5	118.5		5	0.051	58.8	352.8
Ni^{+3}	6	0.056	53.6	160.8		6	0.076	39.5	118.5		6	0.06	50.0	300
Os^{+4}	6	0.063	47.6	190.4	Sb^{+5}	6	0.060	50.0	250.0	Y^{+3}	6	0.09	33.3	99.9
Os^{+5}	6	0.058	51.7	258.5	Sc^{+3}	6	0.075	40.0	120.0		8	0.102	29.4	88.2
Os^{+6}	6	0.055	54.5	327.0		8	0.087	34.5	103.5		9	0.108	27.8	83.4
Os^{+8}	6	0.039	76.9	615.2	Se^{+4}	6	0.050	60.0	240.0	Zn^{+2}	4	0.06	50.0	100
P^{+5}	4	0.017	176.5	882.5	Se^{+6}	4	0.028	107.1	642.6		6	0.074	40.5	81
	6	0.038	78.9	394.5		6	0.042	71.4	428.4		8	0.09	33.3	66.6
Pb^{+2}	6	0.119	25.2	50.4	Si^{+4}	4	0.026	115.4	461.6	Zr^{+4}	4	0.059	50.8	203.2
	8	0.129	23.3	46.6		6	0.04	75.0	300.0		6	0.072	41.7	166.8
	10	0.14	21.4	42.8	Sn^{+4}	4	0.055	54.5	218.0		8	0.084	35.7	142.8
	12	0.149	20.1	40.2		6	0.069	43.5	174.0		9	0.089	33.7	134.8
						8	0.081	37.0	148.0					