Electrical Supplementary Information

Title: Heterogeneous Cu – Pd Binary Interface Boosts Stability and Mass Activity of Atomic Pt Clusters in Oxygen Reduction Reaction

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1. The HRTEM analysis on Cu and Cu@Pd NCs.



Fig. S1. The HRTEM images of (a-1) / (a-2) Cu, (b) Cu@Pd, and Pt/Cu@Pd NCs in different magnifications.

As indicated in **Fig. S1a**, two types of Cu oxide crystals in Cu<sub>2</sub>O and CuO phasesare found in Cu NC. In Cu@Pd NC (**Fig. S1b**), presence of twin boundaries (arrow A), truncations (dashed arrows), dislocations, and varies d-spaces at (111) facets suggest

the formation of incoherent interfaces between Cu and Pd crystal. In the meantime, the particle size is significantly reduced by ~50 nm as compared to that of Cu NC. The phenomena mentioned above indicate the strong confinement effects of Pd shell crystal in the growth of Cu@Pd NC. For Pt/Cu@Pd, presence of high roughness surface (i.e., substantial increased diffusion scattering in XRD pattern) is consistently revealed by HRTEM. As shown in **Fig. S1b** (HRTEM images at 8M and 4M magnifications), Cu@Pd is grown in an average size of 8 to 10 nm that containing smoothly arranged atomic structure in outmost surfaces (denoted by yellow dashed arrows). On the other hand, truncated facets with high roughness surface are found in Pt capped Cu@Pd NP (**Fig. S1c**). This characteristic can be rationalized by pathways of atomic relocation by galvanic replacement at corner or inter-faceted sites (between Pt<sup>4+</sup> ion and Pd or Cu metal) and subsequent nucleation and crystal growth of Pt clusters in heterogeneous surfaces.



2. X-ray powder diffraction analysis on crystal structure of experimental NCs

Fig S2. XRD patterns of (S2a) Pt-CNT, Pd-CNT, Cu-CNT, and Cu@Pd NCs and (S2b)Pt/Cu@Pd, Cu@Pd, and Pd@Pt NCs. The spectra were measured under the incident X-ray at 18 keV.

As indicated in Fig. S2a, peaksX1 and X2 refer to diffraction lines of (111) and (200)

facets of metallic Pt phase in Pt-CNT crystal. For Pd-CNT, the asymmetry peak profile accounted for formation of PdO phase. In Cu-CNT spectrum, the three sharp peaks at 16.125, 18.639, and 19.017° refer to diffraction lines of Cu<sub>2</sub>O (111), Cu<sub>2</sub>O (110), and CuO (111) with an average grain size of 388.5, 399.1, and 143.9 Å, respectively. For Pd@Pt, compared to that of Pd-CNT, larger extent of peak upshift at X2 reveals the higher extent of Pd-to-Pt intermix at (200) facets. Such an uneven intermix / expansion is understandable due to easy intercalation of Pt atoms in opened surfaces. Meanwhile, broadened peak with increased background diffusion scattering hump at peak region are caused by increasing surface roughness of NC. Such phenomena explain the intercalation of atomic Pt clusters into near-surface region of Pd@Pt NC. Shown in **Fig. S2b**, substantial upshift of (111) and (200) peaks indicate the strong lattice compression in Pt/Cu@Pd NC. For Cu@Pt, significant suppression on peak intensities indicate the strong confinement effect on Cu crystal growth by adjacent to Pt crystal. The splitting of main diffraction line indicates the formation of Cu<sub>3</sub>Pt alloy.

Nanostructure of Pd@Pt is featured by their XRD patterns. To clarify crystal structure information, transmission of experimental samples (i.e., amounts of sample been exposed to incident X-ray) is adjusted to the same value (denoted by the background intensity of patterns at  $15^{\circ}$  and  $23^{\circ}$  in 20 where intensity is contributed only from the scattering interferences between incident X-ray and amount of exposed substance).

According to Fig. S3a, diffraction pattern of Pd-CNT samples is a summation of outgoing X-ray waveforms from metallic Pd (I Pd), surface Pd oxide (I PdOx), and surface roughness (I Q1); where peaks X1 and X2 are (111) and (200) diffraction line of metallic f.c.c. Pd crystal. Compared to that of Pd-CNT (Fig. R3a), X1 and X2 lines are shifted to high angle as a result of interatomic intermix between Pt and Pd atoms in Pd@Pt. Such a phenomenon could be attributed to a Pt intercalation in Pd crystal which increases oxidation of Pd atoms in Pd@Pt (also proved by XAS analysis in ESI, Fig. S4, S5). In addition to peak shift, broadened X1 and X2 peak width  $(W_{Pd@Pt})$  and lifted background (shoulder Q) suggest the presence of diffuse scattering waves from Pd@Pt NP surface. Those diffuse scatterings (i.e., I Q2 in Fig. S3a) could be attributed to interactions between incident X-ray and the high roughness or heterogeneous interfaces (i.e., Pt – Pd interface or Pd topmost surface) of Pd@Pt NPs. Identical phenomenon is found when capping Pt atoms in Cu@Pd NP. Shown in Fig. S3b, intensity of X1 and X2 diffraction lines of Pt/Cu@Pd is substantially decreased by more than 40% as compared to that of Cu@Pd. Such a characteristic implies a dramatic decrease of long-range ordering structure (scattering mass<sup>1</sup>) due to

intercalation of Pt clusters in Pd region and surface of Pt/Cu@Pd. Again, observed characteristics can be rationalized by splitting of outgoing X-ray photon flux to diffuse scattering angles (I\_Q2) in a presence of heterogeneous interface (Pt clusters in Pd) and reducing of ordered metallic crystal domain (Cu3Pd and Pd) due to relocations between Pt and Pd, Cu atoms.

The presence of high roughness surface (i.e., substantial increased diffusion scattering in XRD pattern) is consistently revealed by HRTEM images (**Fig. S1**). As shown in **Fig. S1b** (HRTEM images at 8M and 4M magnifications), Cu@Pd is grown in an average size of 8 to 10 nm that containing smoothly arranged atomic structure in outmost surfaces (denoted by yellow dashed arrows). On the other hand, truncated facets with high roughness surface are found in Pt capped Cu@Pd NP (**Fig. S1c**). This characteristic can be rationalized by pathways of atomic relocation by galvanic replacement at corner or inter-faceted sites (between Pt<sup>4+</sup> ion and Pd or Cu metal) and subsequent nucleation and crystal growth of Pt clusters in heterogeneous surfaces.

In addition to structural information mentioned above, growth mode of Pd crystal in Cu@Pd NP is further revealed by XRD and HRTEM analyses. As indicated by XRD patterns in **Fig. S3a**, substantially decreased peak intensity at 16.2° illustrating the suppression of Cu<sub>2</sub>O growth by a subsequent reduction of Pd crystal in Cu NP surface of Cu@Pd. Such a phenomenon is consistently revealed by absence of large Cu oxide particles in HRTEM image of Cu@Pd (**Fig. S1b**). Given that offset of X1 and X2 peak position is nearly absence, formation of CuPd alloy is not considered. In such a case, formation of homogenous alloy will not substantially reduce the long-range ordering of NP (i.e., diffraction peak intensity) but shift diffraction peaks to high angle side due to the formation of Cu alloy in Pd crystal (or to the opposite). On the other hand, observed diffraction peaks with broadened width can be explained by growing Pd crystal in Cu surface; where certain extent of Pd-Cu alloy occurred in interface region.



Fig. S3 XRD patterns of CNT supported (a) Pt, Pd, and Pd@Pt NPs and (b) Cu, Cu@Pd, and Pt/Cu@Pd NPs; where peaks X1 and X2 refer to diffraction lines of f.c.c. metals (Pt or Pd).

| NC     | component          | 20     | index | D <sub>avg</sub> (Å) | $d_{(hkl)}(\text{\AA})$ | ε vs.  | ε vs.  | ref       |
|--------|--------------------|--------|-------|----------------------|-------------------------|--------|--------|-----------|
|        |                    |        |       |                      |                         | Pd (%) | Pt (%) |           |
| Cu-CNT | Cu <sub>2</sub> O  | 16.125 | (111) | 388.5                | 2.482                   |        |        | mp-361    |
|        |                    | 18.639 | (110) | 399.1                | 2.149                   |        |        |           |
|        | CuO                | 19.017 | (111) | 143.9                | 2.107                   |        |        | mp-14549  |
| Pd-CNT | Pd                 |        | (111) | 74.6                 | 2.304                   | 0.96   |        | mp-2      |
|        |                    |        | (200) | 78.3                 | 1.972                   | -0.25  |        | mp-2      |
|        | PdO                |        | (200) | 87.7                 | 2.274                   | 0.04   |        | mp-10728  |
|        | PdOx               |        | (220) | 37.2                 | 2.011                   | 1.98   |        | mp-2      |
| Pt-CNT | Pt                 |        | (111) | 51.0                 | 2.273                   |        | 0.35   | mp-126    |
|        |                    |        | (200) | 42.1                 | 1.972                   |        | 0.51   |           |
| Pd@Pt  | Pt                 |        | (111) | 47.4                 | 2.273                   | -0.39  | 0.35   | mp-126 /  |
|        |                    |        |       |                      |                         |        |        | mp-2      |
|        |                    |        | (200) | 50.4                 | 1.976                   | -0.05  | 0.71   |           |
| Cu@Pd  | Pd                 |        | (111) | 63.9                 | 2.258                   | -1.05  |        | mp-2      |
|        |                    |        | (200) | 52.4                 | 1.949                   | -1.22  |        | mp-2      |
|        | Cu <sub>3</sub> Pd |        | (111) | 75.9                 | 2.223                   | 3.63   |        | mp-580357 |
| Cu@Pt  | Pt                 | 17.728 | (111) | 54.8                 | 2.259                   |        | -1.72  |           |
|        |                    | 20.58  | (200) | 32.0                 | 1.949                   |        | 2.15   |           |
|        | Cu <sub>3</sub> Pt | 18.217 | (111) | 28.1                 | 2.199                   |        |        | mp-12086  |
|        |                    | 21.206 | (200) | 35.7                 | 1.892                   |        |        |           |

Table S1 XRD determined structure parameters of experimental NCs

|          | Cu <sub>2</sub> O  | 16.261 | (111) | 297.7 | 2.461 |       |       |
|----------|--------------------|--------|-------|-------|-------|-------|-------|
|          |                    | 18.792 | (200) | 318.4 | 2.132 |       |       |
| Pt/Cu@Pd | Pt                 | 17.753 | (111) | 67.5  | 2.256 | -2.06 | -1.32 |
|          |                    | 20.601 | (200) | 34.5  | 1.947 | -1.51 | -0.76 |
|          | Cu <sub>3</sub> Pd | 18.146 | (111) | 47    | 2.207 |       |       |
|          | Pd                 | 20.108 | (200) | 598.7 | 1.994 |       |       |
|          |                    |        |       |       |       |       |       |

Table S2 Experimental surface energy ( $E\gamma$ ) of metallic Cu, Pd, and Pt crystal at difference facets.

| metal | Structure   | Surface | FCD                      | FCD                  | FP                   | Experimental         |
|-------|-------------|---------|--------------------------|----------------------|----------------------|----------------------|
| _     | (a(Å))      |         | (eV atom <sup>-1</sup> ) | (J m <sup>-2</sup> ) | (J m <sup>-2</sup> ) | (J m <sup>-2</sup> ) |
| Pt    | fcc (4.109) | (111)   | 1.004                    | 2.299                | 2.067a               | 2.489b, 2.475b       |
|       |             | (100)   | 1.378                    | 2.734                |                      |                      |
|       |             | (110)   | 2.009                    | 2.819                |                      |                      |
| Pd    | fcc (3.985) | (111)   | 0.824                    | 1.92                 | 1.64                 | 2.003, 2.050         |
|       |             | (100)   | 1.152                    | 1.152                | 1.86, 2.3,           |                      |
|       |             |         |                          |                      | 2.130                |                      |
|       |             | (110)   | 1.559                    | 1.559                | 1.97, 2.5            |                      |
| Cu    | fcc (3.661) | (111)   | 0.707                    | 1.952                | 1.94                 | 1.790, 1.825         |
|       |             | (100)   | 0.906                    | 2.166                | 1.802                |                      |
|       |             | (110)   | 1.323                    | 2.237                |                      |                      |

#### 2. X-ray absorption spectroscopy inspection

As shown in Fig. S3 (Pt  $L_3$ -edge XANES), reflection points for the peak maximum (arrow A) at 1<sup>st</sup> deviation spectra of Pt-CNT and Pt foil are located in the same place. Such a characteristic depicts the identical chemical state of the two sample.

Figure S4 (a) and (b) demonstrate the Pd K-edge XANES and radial function of experimental NCs. As can be seen in Fig. S4a inset, the upshift of reflection points J and K to high energy side are indication for the electron relocation to neighboring atoms in Pt/Cu@Pd. Further evidence to such a hypothesis is given by the absence of surface oxygen chemisorption peak in radial function (peak M) in Fig. S4b.



Fig. S4 Pt L<sub>3</sub>-edge XANES spectra of Pt-CNT and standard Pt foil.



Fig. S5 Pd K-edge (a) XANES spectra and (b) Fourier transformed EXAFS spectra (radial function) of experimental samples.

# 3. A single oxygen atom adsorption on Pt<sub>4</sub>-Cu(111) and Pt<sub>4</sub>-Pd/Cu(111) surfaces by using density functional theory.

For a single oxygen atom adsorption on a Pt<sub>4</sub> embedded in a fcc(111) surface, there are eight possible different adsorption sites which are two top, three bridge, and three hollow sites (Pt-TOP and Pd-TOP refer to the oxygen adsorption sites atop Pt and Pd atoms. BRI-1, BRI-2, and BRI-3 stand for the bridge sites between two Pd-top atoms in the vicinity of one Pt atom, Pt dimmer, two separated Pt atoms in the second layer, respectively. Regarding the three hollow site, FCC1 and FCC2 are defined as the oxygen adsorbed on the FCC site with and without forming a Pt-O bond; HCP refers to the oxygen adsorption energy of an oxygen atom on these three models, the reference energy of an oxygen atom is the half of the energy of an oxygen molecule. Table S3 shows the same trend of the greatest O adsorption strength on hollow site. Compared to Pt<sub>4</sub>-Pd/Cu(111) and Pt<sub>4</sub>-Cu(111)systems, the more negative O adsorption energy implies the stronger oxidation capability in the latter system.

|        | E <sub>ads</sub> (eV)       |                          |  |  |  |  |  |
|--------|-----------------------------|--------------------------|--|--|--|--|--|
| Site   | Pt <sub>4</sub> -Pd/Cu(111) | Pt <sub>4</sub> -Cu(111) |  |  |  |  |  |
| Pt-TOP | -0.25                       | -0.34                    |  |  |  |  |  |
| Pd-TOP | 0.39                        | NA                       |  |  |  |  |  |
| Cu-TOP | NA                          | 0.18                     |  |  |  |  |  |
| FCC1   | -1.25                       | -1.64                    |  |  |  |  |  |
| FCC2   | -1.27                       | -1.85                    |  |  |  |  |  |
| НСР    | -0.95                       | -1.63                    |  |  |  |  |  |

Table S3 Oxygen adsorption energy at possible adsorption sites in the models of  $Pt_4$ -Pd/Cu(111) and  $Pt_4$ -Cu(111).

## 4. Electrochemical inspection on NC in ORR

Figure S5a and S6b compares the LSV and CV curves of control samples (JM-Pt, CNT, Cu-CNT, Pt-CNT, Pd-CNT, and Cu@Pd NCs) in ORR. The electrolyte is a basic solution of 0.1M KOH water solution. As shown in Fig. S5a, on-set voltage ( $V_{OC}$ ) and mass activity (MA) of the four NCs follow the trend of JM-Pt > Pt-CNT >Cu@Pd>Pd-CNT. The former represents activation energy and the latter implies reaction kinetics of the NC under-investigation. According to Fig. S6b, the strongest Pd-O reduction peak indicates the highest ESCA of Cu@Pd among experimental NCs. Given that the specific surface area of Cu@Pd is 35% higher than that of Pd-CNT, the dramatic increased ESCA by 400% declares that the majority Pd atoms of Cu@Pd NC are exposed to electrolyte. Such a feature further confirms the confinement effect of Pd shell crystal on Cu@Pd crystal growth by allocating Pd atoms in the surface of Cu crystal. The mass activity (MA) of the catalysts are obtained by using the following equation:

## $MA = I_{0.85} / [Pt]$

where  $I_{0.85}$  represented the current density at 0.85 volt vs. RHE and [Pt] represented the Pt loading (mg cm<sup>-2</sup>) in the electrode.



Fig. S6 (a) LSV of JM-Pt, Pt-CNT, Pd-CNT, Cu@Pd, CNT, and Cu-CNT and (b) CV of JM-Pt, Pt-CNT, Pd-CNT, and Cu@Pd control samples.

| NC     | V <sub>OC</sub> | n   | ECSA                                     | $\mathbf{J}_{\mathbf{k}}$ | S.A.                   | MA                       | MA                       |
|--------|-----------------|-----|--|---------------------------|------------------------|--------------------------|--------------------------|
|        | (vs. RHE)       |     | (cm <sup>2</sup> mgPd+Pt <sup>-1</sup> ) | (mA cm <sup>-2</sup> )    | (mA cm <sup>-2</sup> ) | (mA mgPt <sup>-1</sup> ) | (mA mgPd <sup>-1</sup> ) |
| JM-Pt  | 0.922           | 4   | 270.3                                    | 5.34                      | 0.248                  | 67.1                     |                          |
| Pt-CNT | 0.882           | 3.9 | 79.75                                    | 3                         | 0.41                   | 32.7                     |                          |
| Pd-CNT | 0.854           | 3.8 | 107                                      | 0.741                     | 0.0753                 |                          | 8.1                      |
| Cu@Pd  | 0.869           | 3.6 | 503.3                                    | 1.82                      | 0.0163                 |                          | 8.19                     |

Table S4 Electrochemical performances of control samples in ORR



5. HRTEM investigation on Post ADT NC

Fig. S7 HRTEM images of (S7a) Pt/Cu@Pd, (S7b) Pd@Pt, and (S7c) Cu@Pt NCs. Insets (1) and (2) denote the EDX spectra of NC at assigned positions in HRTEM images.

As indicated in S7, necking between particles with dramatic particle size variations indicate that metal dissolution is the main reason for the current degradation of NC in ADT. In addition, one can note that configuration of heterojunction predominates the reaction pathways. For Pt/Cu@Pd NC, agglomeration of large particles into interconnected crystal is found where small particles well dispersed in CNT (Fig. S7a). From EDX analysis, small particle contains mainly Pt and Cu. It indicates the dissolution of Pd and formation of PtCu alloy by retained metal. The large interconnected particles have higher Pd contents than Pt and Cu. This phenomenon reveals the relocation of Pd into large particle in carbon support. For Pd@Pt NC (Fig. S7b), significant loss of Pd is found in individual particles on CNT indicating the dissolution domination on current density degradation. In Cu@Pt, all NC keep an

average size  $\sim$ 5 nm after ADT (Fig. S7c). Necking between NC reduces the specific surface area and thus the current density in ADT. The Pt/Cu ratios remain unchanged suggesting the absence of selectivity issue between Pt and Cu upon dissolution of NC in ADT.

## 6. Electrochemical analysis on NCs during ADT



Fig. S8 CV sweeping curves of (a) Pt/Cu@Pd, (b) Pd@Pt, (c) Cu@Pt, (d) Cu@Pd NCs, (e) commercial Pt catalyst (J.M.-Pt/C) and (f) changes of onset voltage ( $V_{OC}$ ) for the five samples with increasing ADT cycles.

Fig. S8 demonstrates CV sweeping curves of experimental after ADT at different cycles; where two pairs of redox peaks A / A\* and B / B\* refer to adsorption / desorption currents from oxygen / hydrogen atoms atop NC reaction sites. As indicated in Fig. S8a, the two highly symmetry redox peaks A / A\* and B / B\* with position and intensity indicate the reversible chemical states of Pt/Cu@Pd in CV cycles. In this event, changes of peak position and intensity symmetrically with increasing ADT cycles confirm its strong electrochemical stability in long-term ORR. For Pd@Pt (Fig. S8b), asymmetry peaks A and A\* reveal the irreversible redox reaction at Pd phase. It features the decreasing Pd metal via formation of PdO followed by dissolution due to the fact forreaction kinetics of Pd reduction is substantially lower than that of Pd oxidation formation and corrosion in ORR. Similar characteristics occur in Cu@Pt and Cu@Pd NCs. For Cu@Pt (Fig. S8c), CV sweeping curve is substantially modified by ADT for 1000 cycles. It indicates the completely difference of surface chemical state on NC due to the corrosion of Cu oxide phases in Cu@Pt NC in the first 1000 cycles. After that, intensity of peak B / B\* is progressively decreased by ~25-30% which results in the same fading ratio of residual current till 7000 cycles. Cu@Pd shows similar CV profile to that of Pt/Cu@Pd but in an absence of Hads / Hdes peaks. By increasing ADT cycle numbers, intensity of peaks A and A\* are progressively fading with positions shift to opposite sites. These characteristics indicate the dramatic Pd oxidation and dissolution in long-term ORR. On the other hand, such an electrochemical response provides a control evidence to the protection effect of atomic Pt clusters on Pt/Cu@Pd NC in redox system.

# 7. Reaction kinetics inspection by Tafel plot analysis



Fig. S9 Tafel plot of experimental NCs in ORR.

As demonstrated in Fig. S9, the lowest over-potential decade suggesting the highest corrosion resistance of Pt/Cu@Pd among experiment NCs. In the meantime, the highest exchange current of Pt/Cu@Pd reveals its highest intrinsic reaction kinetics for ORR.

# 8. Structure and electrochemical analysis for cross-referencing inspection on reaction pathways of NC in ORR

|              | XRD analysis     |                  | LSV analysis          |                |                |               |                       |                       |  |
|--------------|------------------|------------------|-----------------------|----------------|----------------|---------------|-----------------------|-----------------------|--|
| NC           | D <sub>avg</sub> | TSA              | ECSA                  | $J_k$          | $\Delta J_k$   | $\Delta J_k$  | MA                    | MA                    |  |
|              | (111) (nm)       | $(m^2 g^{-1})^*$ | $(cm^2 mgPd+Pt^{-1})$ | $(mA cm^{-2})$ | vs. Pd-CNT (%) | vs. JM-Pt (%) | mA mgPt <sup>-1</sup> | mA mgPd <sup>-1</sup> |  |
| Pt-CNT       | 5.1              | 223.1            | 79.75                 | 3.00           |                | -43.8         | 32.7                  |                       |  |
| Pd-CNT       | 7.46             | 267.6            | 107                   | 0.74           |                | -86.1         |                       | 8.1                   |  |
| <u>Cu@Pd</u> | <u>6.39</u>      | 358.7            | 503.3                 | 1.82           | 145.95         | -65.9         |                       | 8.19                  |  |
| Pd@Pt        | <u>4.74</u>      | 358.7            | 300.8                 | 8.19           | 1006.76        | 53.4          | 91.3                  |                       |  |
| <u>Cu@Pt</u> | <u>5.48</u>      | 373.4            | 617.7                 | 2.84           |                | -46.8         | 20.4                  |                       |  |
| Pt/Cu@Pd     | <u>6.75</u>      | 299.9            | 727                   | 21.90          | 2859.46        | 310.1         | 414                   |                       |  |
| JM-Pt        |                  |                  | 270.3                 | 5.34           |                | NA            | 67.1                  |                       |  |

Table S5 XRD and electrochemical characterization determined structure parameters of experimental NCs

\* Theoretical surface area of NC: specific surface area of NC determined by average particle size of NC

TSA can be determined by following numerical representations:

→ To simplify the estimation, NCs are draw as a hard-sphere particle in a surface area of  $A_{NC} = 4 \times \pi R_{NC}^2$ ; where  $R_{NC}^2$  denotes the radius of particle. Consider aspherical particle with adiameter of  $D_{avg}$ , the  $R_{NC}$  should be presented as  $D_{avg}/2$ . Accordingly, volume of each NC is derived as  $V_{NC} = 4 \times \pi (\frac{D_{avg}}{2})^2$  and thus the weight of each particle is represented as  $M_{NC} = V_{NC} \times \rho_{NC}$ . In this equation,

 $\rho_{NC}$  denotes the mass density and volume of individual particle. Consequently, the theoretical specific surface area (TSA) per gram of NCs could be estimated by adopting the density of Pt, Pd, and Cu into following equation:

$$TSA = \frac{1}{M_{NC}} \times A_{NC} = \frac{A_{NC}}{V_{NC} \times \rho_{NC}} = \frac{1}{\sum_{i} x_{i} \times \rho_{i}} \frac{A_{NC}}{V_{NC}} \dots (S1)$$

where mass density  $M_{NC}$  is estimated by considering the weighting  $(x_i)$  of *i* metal components in NCs (for example:  $\rho_{NC}$  is a summation of selected *i*metal fraction " $x_i$ " multiplied by its own density  $\rho_i$ .)

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