Nature-inspired electrocatalysts and devices for energy conversion

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Electronic Supplementary Information

S1. "Murray"-inspired materials: derivation of their design equations

According to Murray's law, the cube of the diameter of the parent vessel (d_p) is equal to the sum of the cubes of the diameters of the daughter vessels ($d_i, i = 1 \ldots n$, where n is the number of macro-, meso-, or nano-pores in each particle) at each level of bifurcation[1-3]:

$$d_p^3 = \sum_i^n d_i^3 \qquad [S1]$$

or, in generalized form

$$d_p^\alpha = \sum_i^n d_i^\alpha \qquad [S2]$$

where α is proposed to be equal to 2 for mass or ionic transfer, and 3 for laminar flow.[4]

To obtain a relationship between the macro- and meso-pores of the catalyst, a generalized form of Murray's law is applied, with α = 2:

$$d_{macro}^{\alpha} = \sum_i^n d_{meso,i}^{\alpha} \ or \ d_{macro}^{2} = \sum_i^n d_{meso,i}^{2} \qquad [S3]$$

where d_{macro} and d_{meso} are the diameters of macro- and meso-pores, respectively. The exchange surface area of the macropores is ignored, since it is negligible compared to the total surface area of the material that contains a large number of meso and micropores as well.[4]

To connect meso- to micro-pores, the exchange surface area from mesopores and micropores, along with the mass loss ratio (M_{loss}), cannot be ignored; the latter is proposed to be $M_{loss} = (S_{macro})/(S_{macro} + S_{meso} + S_{micro}) \ll 1$ (where S_{macro}, S_{meso}, and S_{micro} are the specific surface areas of macro-, meso-, and micro-pores, respectively). By applying the law of mass conservation, we obtain:

$$\dot{m}_p - M_{loss} \cdot \dot{m}_p = \sum_{i}^{n} \dot{m}_i \quad [S4]$$

where $\dot{m}_p$ and $\dot{m}_i$ are the mass flows through parent and daughter vessels, respectively. By applying Fick's law, the above equation [S4] is deduced to:

$$d_{meso}^{\ 2} = \frac{1}{1 - M_{loss}} \cdot \sum_{i}^{n} d_{micro}^{\ 2} \quad [S5]$$

References

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