

Supplementary data

Extraction of Se(IV) and Se(VI) from aqueous HCl solution by using a diamide-containing tertiary amine

**Hirokazu Narita^{a,*}, Motoki Maeda^b, Chiharu Tokoro^b, Tomoya Suzuki^a, Mikiya Tanaka^c,
Hideaki Shiwaku^d and Tsuyoshi Yaita^d**

^a Global Zero Emission Research Center, National Institute of Advanced Industrial Science and Technology (AIST), 16-1 Onogawa, Tsukuba, Ibaraki 305-8569, Japan.

^b School of Creative Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku, Tokyo 169-8555, Japan.

^c National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8560, Japan.

^d Materials Science Research Center, Japan Atomic Energy Agency (JAEA), 1-1-1 Koto, Sayo, Hyogo 679-5148, Japan.

(*Corresponding author: hirokazu-narita@aist.go.jp)

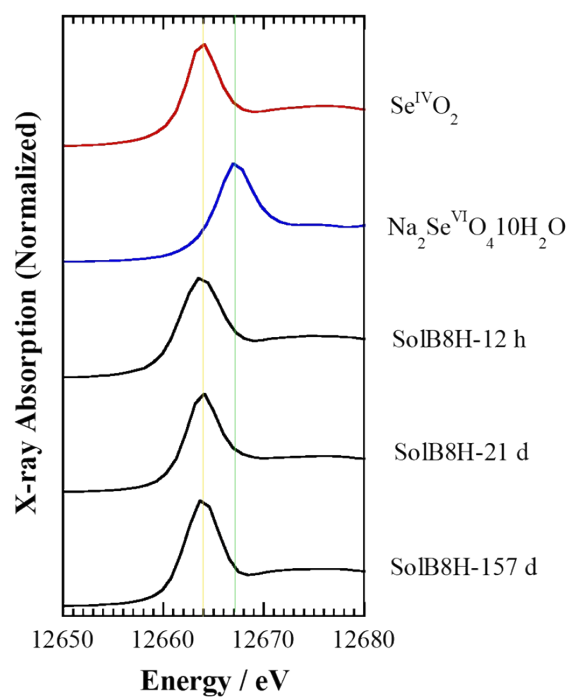


Fig. S1 Effect of standing time (12 h, 21 d, or 157 d) on selenium K-edge XANES spectra obtained for **SolB8H**. **SolB8H** was obtained by dissolving $\text{Na}_2\text{Se}^{\text{VI}}\text{O}_4 \cdot 10\text{H}_2\text{O}$ in 8 M HCl. The solution was then left to stand for the indicated times and then the selenium K-edge XANES spectrum was collected. The spectra for solid samples of $\text{Se}^{\text{IV}}\text{O}_2$ and $\text{Na}_2\text{Se}^{\text{VI}}\text{O}_4 \cdot 10\text{H}_2\text{O}$ are shown for comparison.

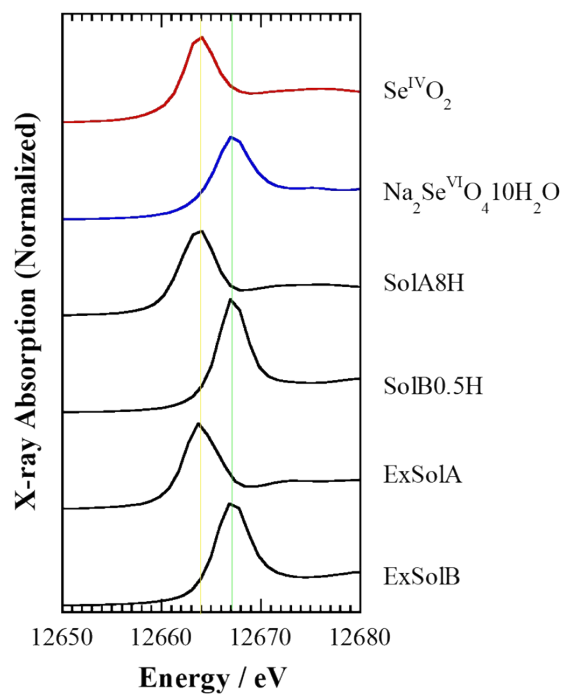


Fig. S2 Se K-edge XANES spectra for the aqueous solutions **SolA8H** and **SolB0.5H**, the organic solutions **ExSolA** and **ExSolB**, and the reference solid ($\text{Se}^{\text{IV}}\text{O}_2$ and $\text{Na}_2\text{Se}^{\text{VI}}\text{O}_4 \cdot 10\text{H}_2\text{O}$).

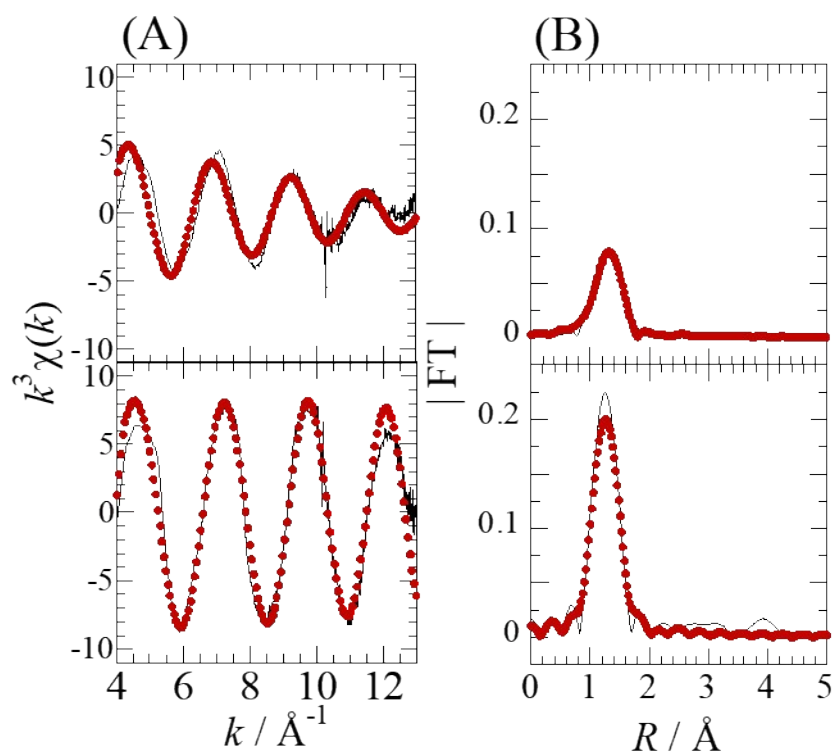


Fig. S3 Se K-edge k^3 -weighted EXAFS spectra (A) and the corresponding Fourier transforms (FT) (B) for the reference solid ($\text{Se}^{\text{IV}}\text{O}_2$ (top) and $\text{Na}_2\text{Se}^{\text{VI}}\text{O}_4 \cdot 10\text{H}_2\text{O}$ (bottom)). The phase shifts are not corrected. Experimental data (solid line) and theoretical fit (dotted line).

Table S1 Curve-fitting results for selenium EXAFS data

| | | N | r (Å) | σ^2 (Å ²) | ΔE (eV) | R-factor |
|--|------|--------|----------|------------------------------|-----------------|----------|
| SeO ₂ | Se–O | 3.1(3) | 1.72(1) | 0.005(1) | 9(1) | 12 |
| Na ₂ SeO ₄ ·10H ₂ O | Se–O | 4.0(4) | 1.645(1) | 0.0005(1) | 6(1) | 8.1 |

The amplitude reduction factor, S_0^2 was fixed at 0.86. N : Coordination number; r : Bond distance (Å); σ^2 : Debye-Waller factor squared (Å²); ^d ΔE : The shift in threshold energy(eV); R-factor = $\Sigma|k^3\chi(k)_{\text{obs}} - k^3\chi(k)_{\text{calc}}| / \Sigma|k^3\chi(k)_{\text{obs}}| \times 100$; Estimated errors are shown in parentheses.