

**Figure SXX.** Extended X-ray Absorption Fine Structure (EXAFS) of Pd2+@CITCF-500. (A) Pd-K edge EXAFS for comparison of Pd2+@CITCF-500 and palladium reference chemicals. (B) k2-weighted Fourier transform of the EXAFS function for Pd2+@CITCF-500 (C), (D) Fitting EXAFS result of Pd2+@CITCF-500 with a combination of Pd-S and Pd-O interation mode.

We additionally performed Extended X-ray Absorption Fine Structure (EXAFS) to investigate Pd-S bonding (Figure SXX) of Pd2+@CITCF-500. Comparison of Pd2+@CITCF-500 and the relevant standards in XANES region (X-ray absorption near edge structure) shows remarkable similarity with PdCl2, which demonstrating Pd2+ oxidation state with a similar average local Pd coordination environement (Figure SXX A). R space analysis (Figure SXX B) shows Pd2+ coordinates predominantly with Pd-S/Cl from the appearance of the peak centered at 1.8 Å (not phase corrected). Slightly lower R value would be due to the bonding with light scattering atoms. The fitting result of EXAFS exhibits a high-agreement with a combination of Pd-S and Pd-O interation mode (Figure SXX C and Figure SXX D). This shows that 2.9 ± 0.3 of S atoms coordinated to Pd and 0.8 ± 0.2 of O atoms coordinated to Pd. We speculate the S from trithiocyanurate and the O from the coordinated H2O molecule. The results of the fitting are given in the table below (Table SXX). The R-factor for the achieved fit was 0.009 as reported by Artemis.

**Table SXX.** The fitting result of Pd2+@CITCF-500 with Pd-S and Pd-O mode.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Scattering path | S02 | N | σ2 (Å2) | e0 (eV) | R (Å) |
| Pd-S | 0.880 | 2.9 ± 0.3 | 0.0058 ± 0.001 | 1.5 | 2.31 ± 0.01 |
| Pd-O | 0.880 | 0.8 ± 0.2 | 0.0025 ± 0.001 | 1.5 | 2.05 ± 0.02 |