

## Description of Additional Supplementary Files

**File Name:** Supplementary Movie 1

**Description:** The volume rendering of the Zr1 nanoparticle. The cross sections of this volume are displayed slice-by-slice from bottom to top. The 3D surface rendering shows the contour of the Zr1 nanoparticle.

**File Name:** Supplementary Movie 2

**Description:** Deciphering the crystalline and amorphous structure of the Zr1 nanoparticle. First, the atoms are colored according to the crystalline and amorphous part with green and blue, respectively. Then, the atoms are colored according to the bond orientation order from low (blue) to high (red), with the red-blue colormap. Finally, the nanoparticle is cut to show the inner atomic structure.

**File Name:** Supplementary Movie 3

**Description:** The Zr1 nanoparticle has complicated phases, composing of a central metal grain (in red), crystalline oxide grains (c-ZrO<sub>2</sub>; in green) and an amorphous oxide phase (a-ZrO<sub>2</sub>; in blue).

**File Name:** Supplementary Movie 4

**Description:** The 3D oxidation and atomic concentration maps of Zr1. First, the atoms are colored according to the metal core and oxide shell with red and ivory, respectively. Then, the atoms are colored according to the degree of oxidation from low (deep red) to high (white) with the colormap 'hot'. Finally, the atoms are colored according to the atomic concentration from low (purple) to high (yellow) with the colormap 'viridis'.

**File Name:** Supplementary Movie 5

**Description:** The distribution of all vacancies, nano-pores, and the largest pore, showing from the beginning to the end of the movie, respectively.