

---

## GENERAL INFORMATION

---

Title of Dataset: Atomic models of Pt nanoparticles supported over ceria.

General description: The models represent multiple Pt nanoparticles, which exhibit different shapes and defects, supported over a ceria surface, that in some models have also been modified including steps. Both nanoparticle and support are oriented on the  $[-110]$  zone axis, and the contact plane is (111) for Pt and (111) for CeO<sub>2</sub>.

---

## NAMING CONVENTION

---

The files present the following structure:

MetalX-DX\_Support-DY-[uvw]\_ThA\_xxYyyYzzZ\_xxxslc\_aaaxbbb\_Dfnm

MetalX-DX: Metal indicates the metallic phase; in our case, Pt. Following X represents a number which describes the structure/size of the particle. DX makes a reference to the defect nature:

- D0: no defects
- D1: one atomic column has been removed
- D2: two atomic columns have been removed
- D3: three atomic columns have been removed
- Dh: one atomic column presents half of its occupancy
- Ds: one "atomic column" presents a single atom

SupportY-DY: Support indicates the material where the nanoparticle has been deposited; in our case, CeO<sub>2</sub>. DY indicates the superficial modifications accomplished on the surface:

- Dst0: no structural modifications
- Dst1: a single step has been included in the surface
- Dst3: three steps have been included in the surface, with just a single column length (this modification leads to the generation of a (110) facet)
- Dst3-steps: At least one of the steps present two or more columns length.

[uvw]: zone axis of the support (orientation).

ThA: Thickness of the supercell in angstroms.

xxYyyYzzZ: Rotation in degrees along the X, Y and Z axis.

xxxslc : number of slices

aaaxbbb : size of the image in pixels

Dfnm: Defocus value for the simulation

EXAMPLE: PtNp1-Ds\_ceria1-D0\_[-110]\_30A\_04x00y00z\_180slc\_256x256\_14nmDefocus

PtNp1-Ds : nanoparticle with structure 1 and one atomic column with a single atom

ceria1-D0 : Surface or Seri with no defects

[-110] : orientation of the support

30A : 30A thickness

04x00y00z : the model is tilted 4 degrees in x axis, and no rotation on y and z axis.

180slc : 180 slices

256x256 : image size of 256 per 256 pixels

14nmDefocus : 14 nm of defocus value

---

#### DATA OVERVIEW

---

There are 14 different Pt models (PtNp1-D0, PtNp1-D1, PtNp1-D2, PtNp1-Dh, PtNp1-Ds, PtNp2-D0, PtNp2-D1, PtNp2-Dh, PtNp2-Ds, PtNp3-D0, PtNp3-D1, PtNp3-D2, PtNp4-D0 and PtNp4-D1) and 4 ceria support (ceria-Dst0, ceria-Dst1, ceria-Dst3 and ceria-Dst3-steps). In total, around 100 atomic-scale structural models of CeO<sub>2</sub>-supported Pt nanoparticles were generated. Each model represents Pt nanoparticles of various size, shape and atomic structure (e.g., small, medium, or large size, with either faceted or defected surfaces, or some combination of both), supported on CeO<sub>2</sub>, which itself may present either a faceted surface or one characterized by surface defects. All Pt nanoparticles have been supported over all ceria surfaces

Besides this combination, and to consider a wide range of situations you may face on a real experiment, some other variables have been analyzed:

**Thickness:** The thickness of the CeO<sub>2</sub> support was varied from 3 nm to 6 nm along 1 nm increments. One aspect to note is that the thickness variation is not equally applied to each of the aforementioned models. Variations on thickness leads into modulations of the atomic column's intensities.

**Tilting:** Each resultant model was tilted from 0 to 4

degrees about the x and y axis independently in increments of 1 degree. Thus, variations from 0 in x and 0 in y, to 4 in x and 0 in y or 0 in x and 4 in y were considered.

Defocus: Every model containing a unique shape/structure, thickness, and tilt (855 total) was imaged under a range of defocus values which often arise experimentally. Namely, the defocus was varied from 0 nm to 20 nm, along increments of 1 nm.

Considering all combinations of the varied parameters, a total of 17,955 simulated images were generated for training and testing the neural network

---

#### METHODOLOGICAL INFORMATION

---

The models have been created combining Rhodius and Vesta softwares.

---

#### ADDITIONAL INFORMATION

---

Supercell dimensions have been set to 50Åx50ÅxThickness (30 to 60Å).

Some other important parameters to consider in the simulations have been fixed to a certain value. These parameters are the following:

High tension: 300 kV  
C3: -13 um  
C5: 5 mm  
Spread of focus: 4 nm