Supplemental Information for “Metallic aluminum suboxides with ultra-high electrical conductivity at high pressure”

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Supplemental Method

Details of the high-pressure crystal structure search

We performed fix-composition structure prediction for Al$_2$O$_3$ and variable-composition for Al-O system (from 1:6 to 6:1) at 200 GPa, 500 GPa, 750 GPa, 1 TPa, 1.5 TPa and 2 TPa. When searching for Al$_2$O$_3$, the maximum number of atoms in the unit cell is 30 and when performing variable-composition search, the number is 48. Extensive fix-composition searches were performed for the stoichiometry where a new compound is found in the variable-composition search. In most of the searches, 900 crystal structures (15 generations, 60 structures per generation) were generated for us to select the most stable ones. To accelerate the searching, we added known aluminum oxides structures from previous work as part of initial seeds.

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**Details of the DFT calculations**

We chose $3s^23p^1$ and $2s^22p^4$ as the valence electrons for Al and O while using the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [1]. The plane-wave cutoff was set as 1050 eV and the Brillouin zone (BZ) was meshed choosing the gamma-centered Monkhorst-Pack approximately $2\pi \times 0.025$ Å$^{-1}$. When calculating the electrical conductivity of iron as a comparison, the valence electrons chosen for Fe were $4s^13d^7$ and single particle orbitals were expanded in plane waves with a cutoff of 420 eV. The Brillouin zone (BZ) was meshed choosing the gamma-centered Monkhorst-Pack approximately $2\pi \times 0.03$ Å$^{-1}$ when calculating the transport properties. As for the *ab initio* molecular simulation part, the equations of motion were integrated with ionic time steps of 1 fs and the Brillouin zone was sampled at Γ point only. To ensure the volume of the cell remains reasonable under given pressure, we first run simulations with a $NPT$ ensemble with 2 ps and take the average cell volume of the last 1000 configurations as the volume employed in the $NVT$ simulations.

Due to the existence of the electron localization area in P4/nmm Al$_2$O and P6$_3$/mmc AlO, we need to adjust the Wigner-Seitz radius for each atoms when calculating the electron density of states [2], which is the parameter RWIGS as implemented in VASP code. Here we set RWIGS values in accordance with the results (atomic volumes) of the Bader charge calculations rather than the parameter written in the pseudopotential. The RWIGS for O atoms in P4/nmm Al$_2$O is 1.05 and the RWIGS for Al atoms is 1.2. As for the P6$_3$/mmc AlO, the RWIGS for O and Al atoms are 0.95 and 1.25, respectively.

To validate the dynamical stabilities of the predicted structures, we have investigated the phonon dispersion curves using $2 \times 2 \times 2$ supercells with PHONOPY code [3]. Also, we have investigated the anharmonic phonon dispersion of the Cmcm Al$_4$O$_7$ at 1500 GPa and 300 K using the DynaPhoPy code [4]. The trajectory was provided by the *Ab initio* molecular dynamics simulation with a $2 \times 2 \times 2$
supercell using VASP code.

**Details of the formation energy cross-checks**

We have performed cross-checks for the formation enthalpy of the Al₂O using WIEN2k, VASP and CASTEP software. In the structure searches with AIRSS, the CASTEP code was employed with similar convergence parameters as used in the Vienna *Ab initio* simulation package. For the calculations using WIEN2k code [5,6], the Perdew-Burke-Ernzerhof version of the generalized gradient approximation (GGA-PBE) was employed. For the calculations using VASP code, apart from the GGA-PBE methods, the hybrid exchange-correlation functional (HSE06) [7,8] was applied. For the calculations using CASTEP code [9], similar convergence parameters as used in VASP were employed.
Fig. S1. (a) Enthalpies of the Al$_2$O$_3$ phases relative to the U$_2$S$_3$-type structure in the pressure range from 300 GPa to 2000 GPa. (b) Enthalpies of the Al$_4$O$_7$ phases relative to the Cmcm structure in the pressure range from 800 GPa to 2000 GPa. The crystal structures of the P1 Al$_4$O$_7$ (c) and the Cmcm Al$_4$O$_7$ (d) at 900 and 1500 GPa, respectively. The red and silver spheres denote oxygen and aluminum atoms, respectively.
Fig. S2. Convex hulls for the P4/nmm Al₃O (a), the P6₃/mmc AlO (b), the I₄₁₃d AlO₃ (c), the PT and Cmcm Al₄O₇ structures (d), respectively.
Fig. S3. Convex hulls for the P4/nmm Al₂O using different methods. (a) Perdew-Burke-Ernzerhof version of the generalized gradient approximation (GGA-PBE) was employed using VASP code. (b) Perdew-Burke-Ernzerhof version of the generalized gradient approximation (GGA-PBE) was employed using WIEN2k code. (c) Hybrid exchange-correlation functional (HSE06) was employed using VASP code. (d) Perdew-Burke-Ernzerhof functional was employed using CASTEP code.
**Fig. S4.** Phonon dispersions and electronic band structures of the P4/mbm Al₂O₃ at 1600 GPa. Red and blue lines in Fig. (a) represent the acoustic and optical branches, respectively.

**Fig. S5.** Phonon dispersions and electronic band structures of the P4/nmm Al₂O at 800 GPa. Red and blue lines in Fig. (a) represent the acoustic and optical branches, respectively.
**Fig. S6.** Phonon dispersions and electronic band structures of the P6₃/mmc AlO at 2 TPa. Red and blue lines in Fig. (a) represent the acoustic and optical branches, respectively.

**Fig. S7.** Phonon dispersions and electronic band structures of the I₄₁₃d AlO₃ at 1300 GPa. Red and blue lines in Fig. (a) represent the acoustic and optical branches, respectively.
**Fig. S8.** Phonon dispersions and electronic band structures of the P1 Al₄O₇ at 1000 GPa. Red and blue lines in Fig. (a) represent the acoustic and optical branches, respectively.

**Fig. S9.** Phonon dispersions and electronic band structures of the Cmcm Al₄O₇. (a) Phonon dispersions at 1500 GPa. (b) Phonon dispersions with anharmonic effect at 300 K. (c) Electronic band structures at 1500 GPa. Red and blue lines in phonon dispersions represent the acoustic and optical branches, respectively.
**Fig. S10.** Equation of states (a) and bandgap (b) of the newly found aluminum oxides.
Fig. S11. The projected band structure and the projection of the bands crossing the Fermi level for the P4/nmm Al₂O (a-b) and the P6₃/mmc AlO (c-d) in real space. The cyan triangles, green squares, blue circles and red diamonds in Fig. (a) and (c) represent the contribution of the p and d orbitals of O and Al atoms, respectively. The energy interval chosen in Fig. (b) and (d) is from -0.5 eV to 0.5 eV.
**Fig. S12.** The electrical conductivity versus temperature of the hcp iron at Earth’s core conditions. Results were obtained using 128, 150 and 250 atoms system, using $2 \times 2 \times 2$ k-points and Gamma point only. The black line is fitted from the experimental results by Ohta et al. [10]. The purple diamonds are the experimental results by Zhang et al. [11]. The red triangles are AIMD results from Pozzo and Alfe’s work in 2016 [12]. The orange dash line is DFPT results taking saturation effects into consideration according to Cohen’s data in 2018 [13]. The crosses are extrapolations to this density using the systematics of Stacey and Anderson based on the melting curve [14]. The green stars are experimental results by Bi et al. using shock-wave compression [15].
Fig. S13. Proposed pressure-temperature phase diagrams of aluminum oxides up to 4TPa and 16000K. The I4_3d AlO₃ becomes stable in area II. The U₂S₃-type Al₂O₃ remain stable in area I and II, while the P4/mbm Al₂O₃ become stable in area III. Both the P4/mbm Al₂O₃ and the P6₃/mmc AlO survive in area IV. Blue squares mark out the estimated pressure-temperature conditions at CMB in the solar giant planets (Uranus, Neptune, Saturn and Jupiter), according to the work by Guillot et al. [16].
**Fig. S14.** Results of the variable-compositions structure prediction at 2 TPa. The blue line represents the convex hull. The green points represent the thermodynamically stable structures and the red crosses represent the thermodynamically unstable structures.
**Fig. S15.** The ELF of the I-4_3d AlO₃. The red spheres represent the O atoms and the sliver spheres represent the Al atoms. The green area around the O atoms is the electron localization region.
Table. SI. Bader charges for atoms in the P4/nmm phase Al₂O at 800 GPa.

| #  | X          | Y          | Z          | CHARGE(e) |
|----|------------|------------|------------|-----------|
| O  | 0.00000    | 0.50000    | 0.89054    | 7.722965  |
| O  | 0.50000    | 0.00000    | 0.10839    | 7.733688  |
| Al | 0.50000    | 0.00000    | 0.81633    | 0.718585  |
| Al | 0.00000    | 0.50000    | 0.18343    | 0.718585  |
| isp(X) | 0.00000 | 0.50000    | 0.59184    | 0.884515  |
| isp(X) | 0.50000 | 0.00000    | 0.37106    | 1.340238  |
| isp(X) | 0.00000 | 0.00000    | 0.40816    | 0.884643  |
| isp(X) | 0.50000 | 0.50000    | 0.62523    | 1.328445  |
| isp(X) | 0.00000 | 0.00000    | 0.37106    | 1.339419  |
| isp(X) | 0.00000 | 0.00000    | 0.62523    | 1.329239  |

NUMBER OF ELECTRONS: 24.0000

Table. SII. Bader charges for atoms in the P6₃/mmc phase AlO at 2 TPa.

| #  | X          | Y          | Z          | CHARGE(e) |
|----|------------|------------|------------|-----------|
| O  | 0.00000    | 0.00000    | 0.50000    | 7.887712  |
| O  | 0.00000    | 0.00000    | 0.00000    | 7.887714  |
| Al | 0.66667    | 0.33333    | 0.25000    | 0.814927  |
| Al | 0.33333    | 0.66667    | 0.75000    | 0.814869  |
| isp(X) | 0.33333 | 0.66667    | 0.25000    | 0.027933  |
| isp(X) | 0.66667 | 0.33333    | 0.75000    | 0.027914  |

NUMBER OF ELECTRONS: 18.0000
Table. SIII. Bader charges for atoms in the P6\textsubscript{3}/mmc phase AlO\textsubscript{3} at 1300 GPa.

| #  | X       | Y       | Z       | CHARGE(e) |
|----|---------|---------|---------|-----------|
| O  | 0.035259| 0.830392| 4.308448| 6.800009  |
| O  | 2.857206|-0.830392| 1.415983| 6.788354  |
| O  | 2.857206| 0.830392| 1.476482| 6.792030  |
| O  | 2.927724| 2.062073| 1.476482| 6.796171  |
| O  | 4.308448| 0.035259| 0.830392| 6.800009  |
| O  | 1.415983| 2.857206|-0.830392| 6.788354  |
| O  | 1.476482| 2.857206| 0.830392| 6.792030  |
| O  | 1.476482| 2.927724| 2.062073| 6.793651  |
| O  | 0.830392| 4.308448| 0.035259| 6.800009  |
| O  | -0.830392| 1.415983| 2.857206| 6.788354  |
| O  | 0.830392| 1.476482| 2.857206| 6.792030  |
| O  | 2.062073| 1.476482| 2.927724| 6.793651  |
| O  | 2.276624| 1.481492|-0.030249| 6.800009  |
| O  | 3.508306| 1.410973|-0.030249| 6.788354  |
| O  | 2.276624|-1.481492| 2.922714| 6.792030  |
| O  | 0.615841| 1.481492| 0.030249| 6.793651  |
| O  | 1.481492|-0.030249| 2.276624| 6.800009  |
| O  | 1.410973|-0.030249| 3.508306| 6.788354  |
| O  | -1.481492| 2.922714| 2.276624| 6.792030  |
| O  | 1.481492| 0.030249| 0.615841| 6.796171  |
| O  | -0.030249| 2.276624| 1.481492| 6.800009  |
| O  | -0.030249| 3.508306| 1.410973| 6.788354  |
| O  | 2.922714| 2.276624|-1.481492| 6.792030  |
| O  | 0.030249| 0.615841| 1.481492| 6.793651  |
| Al | 1.393538|-1.393538| 1.498927| 0.618659  |
| Al | 1.498927| 1.393538|-1.393538| 0.618659  |
| Al | -1.393538| 1.498927| 1.393538| 0.618659  |
|    | 1.393538 | 1.393538 | 1.393538 | 0.619372 |
|----|----------|----------|----------|----------|
| Al | 2.945160 | -0.052695| 0.052695 | 0.618659 |
| Al | -0.052695| 0.052695 | 2.945160 | 0.618659 |
| Al | 0.052695 | 2.945160 | -0.052695| 0.618659 |
| Al | 2.839770 | 2.839770 | 2.839770 | 0.619372 |

**NUMBER OF ELECTRONS:** 168.0000
Crystal structure information (CIF file) for all the structures found in this work

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Al1  Al    0.33887  0.16113  -0.00000  0.01267  Uiso   1.00
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Symmetry cell setting: tetragonal

Symmetry equiv pos as xyz:
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 y, x, z
- y, x, -z
- x+1/2, -y+1/2, -z
 x+1/2, y+1/2, -z
 y, -x, z
- y, -x, z
 x, -y, z
- x, y, z
- y+1/2, -x+1/2, z
 y+1/2, x+1/2, z

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Atom site adp type
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    x-y,-y,z
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| Al1  | Al     | 1.00000 | 0.48178 | 0.50000 | 0.01267 | 1.00  |
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O4  O   0.34961  0.50087  0.94728  0.01267  Uiso   1.00
Al1 Al  0.68683  0.76331  0.64425  0.01267  Uiso   1.00
Al3 Al  0.17981  0.76766  0.94728  0.01267  Uiso   1.00
O2  O   0.00000  0.50000  0.50000  0.01267  Uiso   1.00
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| O1   | O      | -0.31044     | -0.68956     | 0.50000      | 0.01267 | 1.00       |
| Al5  | Al     | -0.87209     | -0.12791     | 0.50000      | 0.01267 | 1.00       |
| O5   | O      | -0.78732     | -0.16302     | 1.25000      | 0.01267 | 1.00       |
| Al1  | Al     | -0.35239     | -0.61776     | 1.25000      | 0.01267 | 1.00       |
| O9   | O      | -0.67192     | -0.67192     | 1.07906      | 0.01267 | 1.00       |
| O13  | O      | -0.85737     | -0.85737     | 0.75000      | 0.01267 | 1.00       |

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- Cell length b: 4.5191
- Cell length c: 5.5073
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z+1/2,x+1/2,-y+1/2
z+1/2,x+1/2,y+1/2
| Atom_site_label | Atom_site_type_symbol | Atom_site_f fract_x | Atom_site_f fract_y | Atom_site_f fract_z | Atom_site_U_iso_or_equiv | Atom_site_adp_type | Atom_site_occupancy |
|----------------|----------------------|--------------------|--------------------|--------------------|--------------------------|--------------------|--------------------|
| Al0            | Al                   | 0.00000            | 0.00000            | 0.00000            | 0.00000                  | 1.00               |                    |
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  -x,-x+y,-z
  y,-x+y,-z
  x+y,x,-z
  -y,-x,z
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  -x+y+1/3,y+2/3,z+2/3
  x+1/3,x-y+2/3,z+2/3
| Parameter                  | Value  |
|----------------------------|--------|
| cell_length_a              | 1.7023 |
| cell_length_b              | 1.7023 |
| cell_length_c              | 7.4994 |
| cell_angle_alpha           | 90.0000|
| cell_angle_beta            | 90.0000|
| cell_angle_gamma           | 120.0000|

**Atom Site Data**

| atom_site_label | atom_site_type_symbol | atom_site_fract_x | atom_site_fract_y | atom_site_fract_z | atom_site_U_iso_or_equiv | atom_site_adp_type | atom_site_occupancy |
|-----------------|-----------------------|-------------------|-------------------|-------------------|--------------------------|-------------------|---------------------|
| O               | O                     | 1.3333            | 0.6667            | -0.26134          | 0.00000                  | Uiso              | 1.00                |

**Geometry Data**

| geom_bond_atom_site_label_1 | geom_bond_atom_site_label_2 | geom_bond_distance | geom_bond_site_symmetry_2 | ccdc_geom_bond_type |
|-----------------------------|-----------------------------|-------------------|---------------------------|---------------------|
| O                           | O                           | 1.080             | 16_544                    | S                   |


data_O2-R-3m

_audit_creation_date 2020-10-24
_audit_creation_method 'Materials Studio'
_symmetry_space_group_name_H-M 'R-3M'
_symmetry_Int_Tables_number 166
_symmetry_cell_setting trigonal

loop_
_symmetry_equiv_pos_as_xyz
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  y,x,-z
  x-y,y,-z
  -x,-x+y,-z
  y,-x+y,-z
  x+y,x,-z
  -y,-x,z
  -x+y,y,z
  x,x-y,z
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  -y+1/3,-x+2/3,z+2/3
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_cell_length_a                    1.7023
_cell_length_b                    1.7023
_cell_length_c                    7.4994
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 120.0000

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  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
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  _geom_bond_distance
  _geom_bond_site_symmetry_2
  _ccdc_geom_bond_type
  O      O       1.080   16_544 S
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