

VOLUNTARY EX ANTE TRANSPARENCY NOTICE

Supplies

Directive 2014/24/EU

SECTION I: CONTRACTING AUTHORITY/ENTITY

I.1) NAME AND ADDRESSES

Official name:

Universiteit van Amsterdam

National ID:

34370207

Postal address:

Postbox 200

Town:

Amsterdam

NUTS code:

NL

Postal code:

1000AE

Country:

NL

Contact person:

Jennifer Bruin

Telephone:

-

E-mail:

j.bruin@hva.nl

Fax:

-

Internet address(es)

Main address:

<http://www.uva.nl>

Address of the buyer profile:

<https://s2c.mercell.com/buyer/569>

I.4) TYPE OF THE CONTRACTING AUTHORITY

Body governed by public law

I.5) MAIN ACTIVITY

- Education

SECTION II: OBJECT

II.1) SCOPE OF THE PROCUREMENT

II.1.1) Title

Diffractionmeter - Voluntary ex ante transparency notice

Reference number: -

II.1.2) CPV code(s)

Main code:

38300000 - Instrumenten voor metingen

Supplementary code:

-

II.1.3) Type of contract

Supplies

II.1.4) Short description

We require a powder X-ray diffractometer, delivering data of highest resolution for precise Rietveld refinements in pure K α 1 radiation. After careful and extensive market research, we concluded that the powder diffractometer STOE STADI MP is the only commercially available device that exclusively and fully accomplishes our prerequisites (Annex D1). This voluntary ex ante notice is used to inform economic operators and to provide them with an opportunity to lodge any objections concerning our intention to award the contract to STOE. Operators will have the opportunity, within a period of 20 days from the date of this notice, to lodge their objections via email. Please send an email to aanbestedingen@uva.nl and mention 'Objections STOE' in the subject line of your email. Any potential objections will be taken into consideration. If we do not receive any objections, we will follow the procedure as laid down in this notice, in which case you will lose the right to oppose the procedure.

II.1.6) Information about lots

This contract is divided into lots: no

II.1.7) Total value of the procurement (excluding VAT)

Value: 366 420,00

Currency: EUR

II.2) DESCRIPTION

II.2.1) Title

-

Lot No: -

II.2.2) Additional CPV code(s)

-

II.2.3) Place of performance

NUTS code:

NL NEDERLAND

Main site or place of performance:

Amsterdam

II.2.4) Description of the procurement:

(nature and quantity of works, supplies or services or indication of needs and requirements)

The group of Prof. Isaeva at the University of Amsterdam focuses on detailed crystal-structure determination of inorganic solids with layered structures (van der Waals quantum materials) and is particularly interested in the accurate elucidation of the lattice symmetry and its temperature-dependent evolution as well as in in-situ intercalation and structure evolution in various gas atmospheres. The main challenges are large and sometimes low symmetric unit cells, various stacking sequences and associated disorder, and polymorphic transitions across the temperature scale.

The combination of these challenges makes the analysis of our samples particularly demanding. Different stacking variants of our materials can have vastly different physical properties, thus the ability to discern the synthesized stacking variants, where the highest intensity peaks can lie as close together as $0.2^\circ 2\theta$, and confirm their purity is mandatory. Examples of close lying reflections of different stacking variants are: $28.75^\circ 2\theta$ (107 reflection for MnSb_2Te_4) and $28.51^\circ 2\theta$ (107 reflection for MnSb_4Te_7 – values for $\text{CuK}\alpha_1$), or (007) peak of MnSb_4Te_7 at $26.23^\circ 2\theta$, (0012) peak of MnSb_2Te_4 at $26.18^\circ 2\theta$, and (009) peak of Sb_2Te_3 at $26.36^\circ 2\theta$.

Omnipresent stacking disorder in van der Waals heterostructures severely impacts the quality of Rietveld refinements. Often, single crystals are unavailable, so ab-initio structure solution from powder data is the routine procedure we employ for structure characterization. Our article (Chem. Mater. 2017, 29, 3, 1321–1337) demonstrates a notable difference in the R-indices for the datasets of the same compound Bi_3TeI refined from by SCXRD ($R_{\text{int}} = 0.03$) and by PXRD ($R_p = 0.06$). The IUCr requirement for R_{int} is that it “should normally be considerably less than 0.10”. In view of the above, we require a powder X-ray instrument

with a resolution of $\pm 0.05^\circ$ 2θ , so we can disentangle the effects of disorder without having to account for instrumental inaccuracies and achieve a reliable structure refinement. Simultaneous data collection in a large interval of 2θ values in transmission geometry in a high temperature chamber under protective or reactive gas atmospheres and in Debye-Scherrer geometry is indispensable for studying the processes of intercalation-deintercalation of our van der Waals compounds.

A large detector window as available with the MYTHEN2 1K ($>18^\circ$ 2θ) allows for single shot measurements in the regions most important for our analyses: 1) The peaks important to reliably define the lattice dimensions of the stacking variant we are dealing with are located in a $5 - 15^\circ$ 2θ interval (d-spacings along the stacking direction between ca. 10 and 40 Å); 2) The effects of atomic intermixing which are tied to the elemental composition are most prominent and discernable at large values of 2θ (from 50 to 90° 2θ interval).

Moreover, in combination with the high temperature chamber, this large window will allow us to precisely trace the structure evolution of the intercalates in various gas atmospheres. Since these transitions may happen very quickly (intercalation in solutions they take around 5 min), snapshots of 10 s or less are necessary for measuring the peak shifts and/or splitting. Our preliminary work shows that intercalation leads to changes in the d-spacing of ca. $0.2 - 0.5$ Å, which would affect the reflections at the low 2θ values at most. In all these measurements we must rely on correct intensity distributions over the whole pattern, to be able to quantify the phase composition of our samples, as a difference in phase composition can change the samples Curie temperature by up to 20 K.

To reach the above-described qualifications, we require a powder X-ray diffractometer, delivering data of highest resolution for precise Rietveld refinements in pure Kalphal radiation.

II.2.5) Award criteria

-

II.2.11) Information about options

Options: no

II.2.13) Information about European Union funds

The procurement is related to a project and/or programme financed by European Union funds: no

II.2.14) Additional information:

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SECTION IV: PROCEDURE

IV.1) DESCRIPTION

IV.1.1) Type of procedure

Negotiated procedure without prior publication

IV.1.3) Information about framework agreement

-

IV.1.8) Information about the Government Procurement Agreement (GPA)

The procurement is covered by the Government Procurement Agreement: yes

IV.2) ADMINISTRATIVE INFORMATION

IV.2.1) Previous publication concerning this procedure

Notice number in the OJ S: -

SECTION V: AWARD OF CONTRACT / CONCESSION

Contract No: -

Lot No: -

Title: -

V.2) AWARD OF CONTRACT / CONCESSION

V.2.1) Date of conclusion of the contract/concession award decision:

30/08/2023

V.2.2) Information about tenders

The contract has been awarded to a group of economic operators: no

V.2.3) Name and address of the contractor/concessionaire

Official name:

STOE & Cie GmbH

National ID:

-

Postal address:

Hilpertstrasse 10

Town:

Darmstadt

NUTS code:

DE

Postal code:

64295

Country:

DE

Telephone:

-

E-mail:

-

Fax:

-

Internet address:

-

The contractor/concessionaire is an SME: no

V.2.4) Information on value of the contract/lot/concession (excluding VAT)

Initial estimated total value of the contract/lot/concession:

366 420,00

01/09/2023

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Total value of the contract/lot/concession: 366 420,00

Currency: EUR

V.2.5) Information about subcontracting

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SECTION VI: COMPLEMENTARY INFORMATION

VI.3) ADDITIONAL INFORMATION

Because of the limited amount of characters allowed in the online form, some parts of the explanation will be a shortened version. If you would like to request the full, longer version of the document, please sent an email to aanbestedingen@uva.nl with 'document request diffractometer' as the object of the email.

VI.4) PROCEDURES FOR REVIEW

VI.4.1) Review body

Official name:

District court Amsterdam

Postal address:

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Town:

Amsterdam

Postal code:

-

Country:

NL

E-mail:

-

Telephone:

-

Internet address:

-

Fax:

-

VI.4.2) Body responsible for mediation procedures

-

VI.4.3) Review procedure

Precise information on deadline(s) for review procedures:

-

VI.4.4) Service from which information about the review procedure may be obtained

-

01/09/2023

[I. II. IV. V. VI. D1.](#)

VI.5) DATE OF DISPATCH OF THIS NOTICE

30/08/2023

ANNEX D1 – GENERAL PROCUREMENT: JUSTIFICATION FOR THE AWARD OF THE CONTRACT WITHOUT PRIOR PUBLICATION OF A CALL FOR COMPETITION IN THE OFFICIAL JOURNAL OF THE EUROPEAN UNION

Directive 2014/24/EU

D1.1) Justification for the choice of the negotiated procedure without prior publication of a call for competition in accordance with Article 32 of Directive 2014/24/EU

The works, supplies or services can be provided only by a particular economic operator for the following reason:

- absence of competition for technical reasons

D1.3) Explanation

Please explain in a clear and comprehensive manner why the award of the contract without prior publication in the Official Journal of the European Union is lawful, by stating the relevant facts and, as appropriate, the conclusions of law in accordance with the directive:
Required features:

- a. Pure KAlpha1 radiation: For lower symmetries and samples containing a mixture of stacking variants, pure KAlpha1 radiation avoids additional reflections from KAlpha2, KBeta and higher homologues in the pattern and therefore reduces the number of lines to the crystallographically possible minimum per parity group, both at ambient and variable temperatures.
- b. A small (5 to 20 mm³) and constant (!) sample volume in the beam over the full 2Theta range: -10° to +140° 2Theta (or better, depending on the selected geometry) and during gas flow measurements +1° to +128° 2Theta in Debye-Scherrer / Transmission geometry.
- c. A direct photon counting detector with smallest pixel / strip width smaller than 55 µm and a large simultaneous 2 Theta window >18° 2Theta is mandatory, especially for the time resolved precise data collection at variable temperature and all other non-ambient measurements.
- d. Interchanging from Transmission- to Reflection mode without any impact on the sample: a quick, simple exchange between geometries without change of the diffractometer optics is necessary.

e. Easy access and teaching: Exchange of sample holders and in-operando cells should be quick and easy.

After careful and extensive market research, we conclude the STOE STADI MP to be the only device that exclusively and fully accomplishes these prerequisites:

re. a) The STADI MP with its built in Johann type Ge(111) monochromator enables pure K α 1 radiation for the two requested geometries, Debye-Scherrer / transmission and Bragg-Brentano.

re. b) Using capillaries, the irradiated sample volume stays constant over the full 2 θ range (-10° to $+140^\circ$ 2 θ) without the necessity of automated slits. The gas reaction and heating chamber “HT2” setup uniquely enables measurements in capillaries in various protective gas atmospheres and temperatures. Very small sample volumes can be employed, which is necessary as our intricate syntheses and intercalation experiments only produce small amounts of material and the Debye-Scherrer geometry also here ensures a constantly irradiated sample volume over the whole accessible 2 θ range ($+1^\circ$ to $+128^\circ$ 2 θ). This setup allows high temperature experiments of our samples without the risk of oxidation. Moreover, we will measure the lattice transformations upon the interaction of the intercalates with the gas phase in-situ, which is not accessible in any other instruments. The offered STOE setup enables fast collection of high-resolution data in a unique experimental setup, in which structure evolution under temperature and gas phase can be studied on small amounts of our intercalated samples (5 to 20 mm³) in a broad temperature range from room temperature to > 1800 K and for minimal gas flows of 0.01 to 0.1 l/min. This type of experiment is not possible in typical reflection geometry reaction chambers. STOE is the only manufacturer offering our required solution and these chambers are only available for STOE X-ray diffractometer systems.

re. c) With 50 micrometer, the MYTHEN2 1K detector offers the smallest strip width of all direct photon counting detectors, thus, highest resolution (FWHM smaller than 0.03° 2 θ for the LaB6 110 NIST 660 standard sample) on the setup is reached. The MYTHEN2 1K's large detector window, covering approx. 18.5° 2 θ simultaneously, allows for ultrafast, noise-free, measurements. The MYTHEN detector series is patent protected, and STOE is the only supplier of such detectors integrated into transmission X-ray diffractometers, see appendix 1.

re. d) To switch geometries, only the tube housing is shifted on ultra-high precision rails. Only the focal spot of the monochromator changes, ensuring no loss in instrument precision as no optical element has to be exchanged. The switch is simply done in minutes, without further necessity for realignment.

re. e) STOE is the only X-ray diffractometer manufacturer offering windows on all 3 sides.