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Order no. **ZP/278/009/D/2020**

Gdańsk, 20.03.2020 y.

ANNOUNCEMENT ABOUT CONTRACT AWARD

Employer - Gdańsk University of Technology Faculty of Electronics, Telecommunications and Informatics, acting on the basis of Art. 4d paragraph 1 point 1) the Act of 29 January 2004 Public Procurement Law (i.e., Journal of Laws of 2019, item 1843), informs about the intention to award a contract in the field of science and invites you to submit offers for the supply of specialized quantum simulation software.

1. Detailed description of the subject of the contract:

- 1) The subject of the order is the delivery of package designed for testing the properties of materials using ab-initio methods. From the project's point of view, an important final result of the program's work will be:

At the point of the project, the important end effects of program works are:

- Calculation of Raman polarizability tensors
- Performing of full geometry optimization (cell parameters and atom coordinates)
- The possibility of constant volume or pressure constrained geometry optimization
- Estimation of harmonic vibrational frequencies at Gamma point
- Estimation phonon dispersion using a direct approach (efficient supercell scheme)
- Simulation of IR intensities
- Simulation of Raman intensities
- Calculation of Phonon band structure and DOSs

The package contains the following computational methods implemented:

- Hartree-Fock Theory: Restricted (RHF), Unrestricted (UHF), Restricted-Open (ROHF)
- Density Functional Theory implementation with the following functionals:
 - o Semilocal functionals: local [L], gradient-corrected [G] and meta-GGA (tau-dependent) [T]
 - o Hybrid HF-DFT
 - o Double hybrid functionals: B2-PLYP, mPW2-PLYP, B2GP-PLYP
- DFT-D3 correction for dispersive interactions. Automated, parameter-free implementation
- Composite methods for molecular crystals: HF-3c, PBEh-3c, HSE-3c and B97-3c

Supported Systems: Unix / Linux required Intel MacOSx + MS Windows

Parallel calculations: MPP option required

- 2) CPV code 48461000-7 analytical or scientific software packages.
- 3) The subject of the contract includes delivery to the contracting authority's headquarters: Gdańsk University of Technology, Faculty of Electronics, Telecommunications and Informatics, 11/12 Narutowicza St., 80-233 Gdańsk, building WETI A (No. 41), room 116.
- 4) The object of the contract was determined by indicating objective technical quality characteristics. Any names (trademarks) provided by the contracting authority are exemplary, and their purpose is to specify the

expected standard, whereby the contracting authority allows submission of equivalent bids in the scope of the prepared description of the subject of the contract.

2. Description of how to prepare the offer:

- 1) The offer should be prepared in accordance with the model offer form constituting Annex 1 to the announcement.
- 2) The offer may be submitted in writing or in electronic form. The offer in electronic form must be submitted as a scan of the written form. The offer must contain the signature of the authorized person(s) to act on behalf of the contractor (proxies should be attached to the offer, in accordance with the requirements of the Civil Code). All attachments to the offer constituting statements should also be signed by an authorized representative. The scope of the entrepreneur's representation must result from documents submitted by the contractor.
- 3) The price should be given in the gross amount for the service, including all costs and fees that will arise in connection with the performance of the contract and with the conditions and requirements set by the contracting authority.
- 4) All pages of the offer, as well as the places where the contractor has made changes, should be initialled by the person signing the offer.
- 5) The Contractor submitting the offer should submit it in an opaque, sealed and described envelope "Offer in the proceeding for the supply of specialized quantum simulation software, case reference number: ZZ/278/009/D/2020". The Contractor submitting the offer electronically should enter the following marking in the subject of the e-mail: "ZZ/278/009/D/2020 offer".

3. Description of the method for calculating the offer price.

- 1) The price must be specified in Polish zlotys to two decimal places.
- 2) If an offer is submitted in a currency other than PLN, the offer price will be converted into PLN at the exchange rate of the National Bank of Poland, Table A, applicable on the day set as the date for submission of offers.
- 3) The price should be given in the gross amount for the delivery including all costs and fees that will arise in connection with the performance of the contract and with the conditions and requirements by the customer.

4. Place and deadline for submission of bids:

- 1) The offer should be submitted by 30.03.2020y., by 10:00, in writing to the address: Gdańsk University of Technology Faculty of Electronics, Telecommunications and Informatics, 80-233 Gdańsk, ul. G. Narutowicza 11/12, WETI A building, room 116 or by e-mail to the following address: logistyka@eti.pg.edu.pl.
- 2) The contractor may request the contracting authority to clarify the content of the offer by electronic means to the e-mail address: logistyka@eti.pg.edu.pl.
- 3) Offers sent after the deadline will not be considered.
- 4) The Contractor may change or withdraw his offer before the deadline for submission of bids.

5. Bid evaluation criteria

When choosing an offer, the contracting authority will be guided by the following award criteria: Price - 100%. The contracting authority will award the contract to the contractor who submits an offer meeting all the conditions of the contract and will offer the lowest price. If two or more bids with the same price are submitted, the contracting authority will call the contractors who submitted these bids to submit additional offers within the time limit specified by the contracting authority. Contractors submitting additional bids cannot offer higher prices than those offered in previously submitted bids..

6. The Purchaser reserves the right not to grant or cancel the procedure at any time without giving reasons.

7. Information clause regarding the processing of personal data and the free movement of such data.

In accordance with art. 13 section 1 and 2 of Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016. on the protection of individuals with regard to the processing of personal data and on the free movement of such data and repealing Directive 95/46 / EC (General Data Protection Regulation) (Official Journal EU L 119 of 05/04/2016, p. 1), hereinafter "GDPR",

the contracting authority informs that:

1) the administrator of your personal data is Gdańsk University of Technology with headquarters in Gdańsk (80-233) at 11/12 Narutowicza St.;

2) the personal data protection inspector at the Gdańsk University of Technology is MSc. Paweł Baniel, tel. 58 348-66-29, e-mail: iod@pg.edu.pl;

3) Your personal data will be processed on the basis of art. 6 clause 1 lit. c GDPR for supply of specialized quantum simulation software, No. ZZ/278/009/D/2020, maintained on the basis of art. 4 point 8 of the Act of 29.01.2004 Public Procurement Law (i.e. Dz. U. of 2019, item 1843),

4) recipients of your personal data will be persons or entities to whom documentation of proceedings based on art. 8 and art. 96 section 3 of the Act of 29 January 2004 - Public Procurement Law (Journal of Laws of 2019, item 1843), hereinafter the "PPL Act";

5) Your personal data will be stored in accordance with art. 97 paragraph 1 of the Public Procurement Law, for a period of 4 years from the date of termination of the contract award procedure, and if the duration of the contract exceeds 4 years, the storage period covers the entire duration of the contract;

6) your obligation to provide personal data directly related to you is a statutory requirement specified in the provisions of the PPL Act related to participation in the proceedings for the award of a public contract; the consequences of not providing specific data result from the Public Procurement Law;

7) with regard to your personal data, decisions will not be taken in an automated manner, applying to art. 22 GDPR;

8) you are entitled to:

- based on Article. 15 GDPR, the right to access your personal data concerning;
- based on Article. 16 GDPR, the right to rectify your personal data (*exercise the right for rectification may not result in a change in the outcome of the public procurement procedure or a change in the contractual provisions to the extent not in accordance with the Public Procurement Law and may not violate the integrity of the protocol and its annexes.*);
- based on Article. 18 GDPR, the right to request the administrator to limit the processing of personal data, subject to the cases referred to in art. 18 clause 2 GDPR (*the right to limit processing does not apply to storage, to ensure the use of legal protection measures or to protect the rights of another natural or legal person, or because of important reasons of public interest of the European Union or a Member State*);
- the right to lodge a complaint to the President of the Office for Personal Data Protection, if you consider it, that the processing of your personal data violates the provisions of the GDPR;

9) you are not entitled to:

- in reference to art. 17 clause 3 lit. b, d or e GDPR the right to delete personal data;
- the right to transfer personal data referred to in art. 20 GDPR;
- based on Article. 21 GDPR, the right to object to the processing of personal data, because the legal basis for the processing of your personal data is art. 6 clause 1 lit. c GDPR.

8. Annex to the contract award notice:

1) template for the offer.

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prof. dr hab. inż. Jerzy Wtorek