

RESEARCH AGREEMENT

BETWEEN

SHELL GLOBAL SOLUTIONS INTERNATIONAL B.V.

AND

LEIDEN UNIVERSITY

FOR

QUANTUM CHEMISTRY ON QUANTUM COMPUTERS

Agreement No. CW209026

THIS AGREEMENT IS MADE as of the 11th of October 2018 by:

SHELL GLOBAL SOLUTIONS INTERNATIONAL B.V., a company incorporated under the laws of Netherlands and having its registered office at **Kessler Park 1, Rijswijk, 2288 GS NETHERLANDS**, hereinafter called "**Shell**".

and

LEIDEN UNIVERSITY, a legal entity under the law of the Netherlands and having its registered office at **Rapenburg 70, 2311 EZ Leiden, NETHERLANDS**, hereinafter called "**Research Partner**".

WHEREAS:

- A. Shell wishes to engage the Research Partner for the provision of certain research services in the area of **Quantum chemistry on quantum computers**
- B. The Research Partner is willing to arrange for such a study to be carried out.
- C. The goal of the research is to produce several scientific "**paper**"(s)

NOW THEREFORE IT IS AGREED AS FOLLOWS:

1. DEFINITIONS AND INTERPRETATION

The following expressions shall have the meanings specified:

"**Affiliate**" with respect to Shell means (a) Royal Dutch Shell plc and any entity other than Shell which is at the time in question directly or indirectly controlled by Royal Dutch Shell plc. For the purpose of this definition, a particular entity is (i) directly controlled by another entity or entities if that latter entity owns or those latter entities together own fifty percent (50%) or more of the ownership interest of, or of the voting or contractual rights in, the particular entity; and (ii) is indirectly controlled by an entity or entities if a series of entities can be specified, beginning with that latter entity or entities and ending with the first mentioned entity, so related that each entity of the series (except the latter entity or entities) is directly controlled by one or more of the entities earlier in the series and (b) any company which is managed or operated by Shell or a company as defined above in (a) and/or has a service agreement with a company as defined in (a) above, pursuant to which it pays or recovers on a cost sharing basis a proportion of certain of the costs of Shell or such company pursuant to a cost allocation key;

"**Agreement**" means this agreement including the appendices to this Agreement, as amended, varied or supplemented from time to time pursuant to Clause 24 hereof;

"**Anti-Bribery Laws**" means the United States Foreign Corrupt Practices Act of 1977 and the United Kingdom Bribery Act 2010 (as amended from time to time) and all other applicable national, regional, provincial, state, municipal or local laws and regulations that prohibit the bribery of, or the providing of unlawful gratuities, Facilitation Payments or other benefits to, any Government Official or any other person;

"**Facilitation Payments**" means payments to facilitate or expedite performance of a routine governmental action which is an action which is commonly performed by a Government Official;

"**Force Majeure Event**" means the events qualifying as a Force Majeure Event as expressly set out in the Agreement;

"Government Official" means any official or employee of any government, or any agency, ministry, department of a government (at any level), person acting in an official capacity for a government regardless of rank or position, official or employee of a company wholly or partially controlled by a government (for example, a state owned oil company), political party and any official of a political party; candidate for political office, officer or employee of a public international organisation, such as the United Nations or the World Bank, or immediate family member (meaning a spouse, dependent child or household member) of any of the foregoing;

"Intellectual Property Rights" means patents, trademarks, service marks, (registered or unregistered) rights in any designs, trade or business names, copyright (including rights in computer software), know-how, secret formulae and processes and other proprietary knowledge and information, rights protecting goodwill and reputation, database rights and all rights, applications for the any of the foregoing and forms of protection of a similar nature to any of the foregoing or having equivalent effect anywhere in the world and all rights under licences and consents in respect of any of the rights and forms of protection mentioned in this definition;

"Laws" means all applicable national, municipal or state statutes, ordinances or other laws (including but not limited to Anti-Bribery Laws), regulations, by-laws or any rules, codes or directions or any licence, consent, permit, authorisation or other approval required by any public body or authority, local or national agency, department, inspector, ministry, official or public or statutory person (whether autonomous or not);

"Notice" means a notice, subpoena, order or other legal process, including any request for disclosure of information pursuant to any applicable Freedom of Information legislation;

"Paper" means a paper as described in Clause 9.1;

"Party" means either Shell or the Research Partner as the context requires and "Parties" shall mean Shell and the Research Partner collectively;

"Personal Data" means any information relating to an identified or identifiable individual, unless otherwise defined under applicable law related to the protection of individuals, the processing of such information, and security requirements for and the free movement of such information.

"Purchase Order" means an order by Shell issued to the Research Partner for the respective, purchase of the Study hereunder;

"Related Party" means in relation to a Party or any of its Affiliates;

- (a) any person employed by that Party or its Affiliates;
- (b) any director or other officer of that Party or its Affiliates; and
- (c) any person acting for or on behalf of that Party or its Affiliates;

and "Related Parties" shall mean the plural;

"Research Associate" means the person(s) nominated by the Research Partner in accordance with Clause 3.2;

"Research Partner Personnel" means any individual employed or supplied by Research Partner whether directly or indirectly and assigned to work in connection with the performance of this Agreement whether or not an employee of Research Partner, and includes Subcontractors of Research Partners and their personnel;

"Restricted Jurisdiction" means countries or states that are subject to comprehensive trade sanctions or embargoes, which at the date of execution of this Agreement include the following: Syria, Cuba, Iran and Sudan (as may be amended by the relevant governmental authorities from time to time);

"Restricted Party" means a party (i) targeted by national, regional or multilateral trade or economic sanctions under applicable laws, including, but not limited to, persons designated on the United Nations financial sanctions lists, European Union (EU) or EU member state consolidated lists, U.S Department of the Treasury Office of foreign assets control lists, U.S State Department non-proliferation sanctions lists or U.S Department of Commerce denied persons list, in force from time to time or (ii) directly or indirectly owned or controlled by or acting on behalf of such persons;

"Results" means the results, conclusions, findings, inventions, solutions, specifications, recommendations, software, user manuals, documentation, reports, designs, drawings, data or other information, documents, or materials, which arise or are made or created in the performance of the Study and includes copyright to any copyright protectable work resulting from the Study;

"Shell Monitor" means the person(s) nominated by Shell in accordance with Clause 0;

"Shell Information" means any information or data, whether disclosed in writing, orally or visually, by way of samples, which is received or obtained by the Research Partner either directly or indirectly from Shell and/or an Affiliate of Shell in connection with the Study or under this Agreement;

"Study" means the study having the scope described in APPENDIX I;

"Subcontractor" means any party to a subcontract other than Shell and Research Partner;

"Supervisor" means the person(s) nominated by the Research Partner in accordance with Clause 3.3;

"Thesis" means a thesis written by the Research Associate as described in Clause 9.1;

"Trade Control Laws" means all applicable governmental laws, regulations, decrees and orders governing the export and re-export of goods, technology, software and/or services, including, to the extent applicable, the U.S. Export Administration Regulations administered by the U.S. Department of Commerce, the U.S. trade sanctions legislation administered by the U.S. Department of the Treasury and European Council Regulation 428/2009 and any amendments thereto and any applicable laws whether imposed by public law (including without limitation and any applicable United States, Canadian, European Union, United Nations, or other export control and trade sanctions laws, regulations and administrative requirements;

"Worksite" means all the lands, waters, facilities, properties and any other places including, but not limited to, storage facilities, offshore installations, floating construction equipment, vessels (including the area approved by anchor patterns), offices, workshops, and messing facilities, on, under, in or through which work in connection with the Agreement will be performed by Research Partner and Research Partner Personnel, which are owned and/or operated by Shell and/or Affiliates of Shell.

2. COMMENCEMENT AND DURATION

This Agreement shall come into effect on 1st of October 2018 and, unless terminated earlier in accordance with Clause 13, shall continue in force until 30th of September 2023.

3. PERSONNEL AND LOCATION

3.1 The Research Partner undertakes to carry out the Study with all professional skill, care and diligence.

3.2 The Research Partner shall assign 5.1.2e to work on the Study for the duration of the Study. The Research Associate's contact details are as follows:

5.1.2e

Niels Bohrweg 2
2333 CA Leiden

5.1.2e

5.1.2e@lorentz.leidenuniv.nl

3.3 The Research Partner shall arrange for the work of the Research Associate on the Study to be supervised by 5.1.2e 5.1.2e contact details are as follows:

Instituut-Lorentz, Universiteit Leiden
P.O.Box 9506, 2300 RA Leiden, The Netherlands
Tel: +31-71- 5.1.2e Email 5.1.2e@lorentz.leidenuniv.nl

- 3.4 Shell shall nominate one of its employees to monitor the progress of the Study and to act as contact point with the Research Partner. The initial Shell Monitor shall be [REDACTED] 5.1.2e contact details are as follows:

Shell Technology Center Houston
3333 Highway 6 S., Houston, TX 77082
Tel: +1 281 [REDACTED] 5.1.2e ; Fax: +1 281 [REDACTED] 5.1.2e
Email: [REDACTED] 5.1.2e @shell.com

- 3.5 The Study shall be carried out at designated premises of Research Partner in Netherlands unless otherwise agreed between Shell and the Research Partner.

4. DELIVERABLES

- 4.1 The Research Partner undertakes to arrange for the Supervisor to:
- (a) keep the Shell Monitor fully informed of the progress on the Study by providing final written reports; and
 - (b) provide the Shell Monitor with the Results in the form of written reports at regular intervals to be agreed.
- 4.2 The Research Partner shall ensure that the Shell Monitor receives a copy of the final report of the Study promptly after completion of the Study. Such report shall set out all Results of the Study.
- 4.3 The Research Partner shall supply to the Shell Monitor:
- (a) copies of the object and source code of any software comprised in the Results; and
 - (b) all samples and other materials (other than draft reports) containing Results.

5. PAYMENT

- 5.1 In consideration of the carrying out of the Study, the supply of the Results and the grant of rights to Shell as specified in Clause 8 Shell shall make the of payment of [REDACTED] 5.1.2b, 5.1.2f in several instalments in accordance with APPENDIX II.
- 5.2 Shell shall pay the Research Partner within sixty (60) days (unless otherwise stated by Shell) of receipt by Shell of a correctly prepared and properly supported invoice. Shell reserves the right to pay only the undisputed portion of any disputed invoice. The parties shall endeavour to settle at the earliest possible date any invoicing matters in dispute.
- 5.3 The Research Partner shall state the Agreement number and the Purchase Order number on the invoice and send its invoices to the address specified in the Purchase Order.

6. SUPPLY OF INFORMATION

Shell shall arrange for the disclosure to the Research Partner of such Shell Information as Shell deems necessary to ensure satisfactory progress is made in the Study.

7. CONFIDENTIALITY OBLIGATIONS

- 7.1 The Research Partner undertakes that it shall not, and warrants that the Supervisor and the Research Associate shall not, without the prior written consent of Shell:
- (a) disclose to any third party any Shell Information, however Research Partner may disclose Shell Information to students (i) agreed by Shell in writing in advance to performing work in the Study and (ii) who have signed a confidentiality and restricted use agreement of at least the same restrictions of confidentiality as stated in this Article 7; or
 - (b) use any Shell Information for any purpose other than the Study.
- 7.2 The Research Partner may disclose Shell Information only to those of its employees who:

- (a) have a reasonable need to know and use such information in furtherance of completing the Study;
 - (b) have been informed of the confidential nature of the Shell Information in question; and
 - (c) are bound by obligations no less stringent than those assumed by the Research Partner hereunder.
- 7.3 The obligations in Clauses 7.1 and 7.2 shall:
- (a) not apply to any Shell Information, at the time it is received or obtained by the Research Partner, is lawfully known by the Research Partner without binder of secrecy or is publicly available; and
 - (b) cease to apply to any Shell Information which, after it is received or obtained by the Research Partner:
 - (i) is received by the Research Partner without binder of secrecy from a source free to disclose it other than Shell and/or any Affiliate of Shell;
 - (ii) becomes publicly available other than as the result of a breach of this Agreement;
 - (iii) is approved for release in advance and in writing by an authorised representative of Shell; or
 - (iv) has been approved for publication in accordance with Clause 9.
- 7.4 If the Research Partner receives a notice seeking disclosure of Shell Information, the Research Partner shall immediately notify Shell and the Shell Monitor in order to allow Shell the opportunity to oppose the Notice or to seek a protective order. If requested by Shell, the Research Partner shall co-operate fully with Shell in contesting such disclosure. Except as such demand shall have been limited, quashed or extended, the Research Partner may thereafter comply with such demand, but only to the extent required by law. Where Shell has obtained a protective order, nothing in this Agreement shall be construed as authorising the Research Partner to use in any manner or disclose Shell Information to parties other than such governmental or judicial agency or body beyond the scope of the protective order.
- 7.5 Information shall only be within the exceptions in Clause 7.3 to the extent that the Research Partner can establish the facts with adequate proof.
- 7.6 ~~Specific disclosures made hereunder shall not be deemed to be subject to any of the exceptions in Clause 7.3 merely because they are embraced by general disclosures in the public knowledge or literature or in the possession of the Research Partner, the Supervisor and/or the Research Associate.~~
- 7.7 Any combination of features disclosed hereunder shall not be deemed subject to the exceptions in Clause 7.3 merely because individual features are in the public knowledge or literature or in the possession of the Research Partner, the Supervisor and/or the Research Associate.
- 7.8 A Party shall not, without the specific prior written permission of the other Party, refer in any of its publicity to this agreement or the relationship between Research Partner and Shell or allow others to do so.
- 8. RIGHTS IN RESULTS**
- 8.1 All right, title and interest in and to the Results shall vest in the Research Partner. The Research Partner shall have the exclusive right to file patent applications in respect of inventions embodied in such Results in its own name and at its own expense in such countries as it deems appropriate.
- 8.2 The Research Partner grants and warrants that the Supervisor and/or the Research Associate, as the case may be, grant to Shell from the date any such Results are created an perpetual, irrevocable, worldwide, non-exclusive, royalty-free right to use, disclose to Affiliates of Shell and other third parties with the right of use, reproduce, adapt translate and otherwise exploit and have exploited the Results.

- 8.3 The Research Partner, warranting that it is free to do so, grants Shell a perpetual, irrevocable, non-exclusive, royalty-free, worldwide licence under:
- (a) any Intellectual Property Rights of the Research Partner; and
 - (b) any Intellectual Property Rights of third parties licensed to the Research Partner with the right to grant sub-licences to third parties,
- which are necessary to use or exploit the Results for any purpose with the right to grant sub-licences to Affiliates of Shell and/or and to third parties to use the Results for the operations of Shell, Affiliates of Shell and/or third parties. The Research Partner agrees that it shall not use the Intellectual Property Rights of third parties to carry out the Study where it is not free to provide a sub-licence to Shell as set out in Clause 8.3.2 (b).
- 8.4 The Research Partner shall be solely liable for employee compensation or remuneration due to inventors, other than employees of Shell and Affiliates of Shell, under any intellectual property legislation.
- 8.5 At the request of Shell, such request to be made before expiry of four (4) years from the date of completion or termination of the Study, the Research Partner will offer Shell the right and licence referred to in Clause 8.2 on an exclusive basis on reasonable terms and conditions to be agreed separately between Shell and the Research Partner. Research Partner agrees and warrants that Supervisor and/or the Research Associate, as the case may be, agree to remain in a position to make such offer for said period.

9. PUBLICATIONS BY THE RESEARCH PARTNER

- 9.1 Without prejudice to Clause 7, Shell recognises that the Research Associate and/or the Supervisor may wish to publish some or all of the Results together with any relevant Shell Information as a paper possibly including software within the Research Partner or in the open literature ("Paper") and/or that the Research Associate may wish to submit a thesis containing the Results together with any relevant Shell Information for a higher degree from the Research Partner ("Thesis").
- 9.2 Before publication of any Paper and prior to any submission of any Thesis, the Research Partner shall arrange for the Paper and/or Thesis to be given to Shell. Shell may examine and change the Paper and/or Thesis to enable Shell to protect Shell Information and Intellectual Property Rights comprised in the Shell Information, including taking steps to file an application for patent.
- 9.3 At any time Shell may withhold its consent to the publication of any Shell Information in any Paper and/or Thesis.

10. WARRANTIES

- 10.1 Shell and/or its Affiliates make no representation and give no warranty as to the accuracy of Shell Information and/or as to its satisfactory quality, fitness or suitability for Research Partner's purpose. The Research Partner will receive and use Shell Information at its own risk.
- 10.2 The Research Partner warrants that the Results are the sole and original work of employees or contractors of the Research Partner, the Research Associate and/or the Supervisor and/or students involved in the Study.

11. FORCE MAJEURE

- (a) Shell and Research Partner are each excused from performance of the affected part of an obligation of the Agreement while performance is prevented by a Force Majeure Event unless the event: (i) was contributed to by the fault of the party or was due to circumstances that could have been avoided or mitigated by the exercise of reasonable diligence by (A) any member of Research Partner or its Related Parties where Research Partner claims force majeure or (B) any Affiliate of Shell where Shell claims force majeure; or (ii) relates to an inability to make payments of money or secure funds.

- (b) Only the following are Force Majeure Events: (i) riots, wars, blockades, or acts of sabotage; (ii) threats or acts of terrorism; (iii) radioactive contamination; (iv) earthquakes, floods, fires, named hurricanes or cyclones, tidal waves, tornadoes, or other natural physical disasters; (v) epidemics; (vi) maritime or aviation disasters; (vii) strikes or labour disputes at a national or regional level or involving labour not forming part of Research Partner and its Related Parties or Shell, which materially impair the ability of the party claiming force majeure to perform the Agreement; (viii) government sanctions, embargoes, mandates, or laws, that prevent performance; (ix) inability of a party to obtain licences, permits, or governmental consents required for performance; or (x) non-performance of a party's Subcontractor where the Subcontractor has been or is affected by one of the above Force Majeure Events. However, performance will only be excused under this sub-article if the parties agree that substitute performance by another Subcontractor is impracticable under the circumstances.
- (c) A party whose performance is delayed or prevented will: (i) notify the other party without delay; (ii) use all reasonable endeavours (including acceleration of schedules on resumption of performance) to mitigate the effects; and (iii) provide on a continuing basis plans for resumed performance and revised schedules.
- (d) Shell may terminate the Agreement if any Force Majeure Event results in a delay that exceeds ninety (90) consecutive or one hundred and eighty (180) cumulative days, except where Shell has provided a Purchase Order.

12. RESEARCH PARTNER PERSONNEL AND SUBCONTRACTING

- 12.1 Research Partner is responsible for any Study performed by and all activities, omissions, and defaults of any Subcontractor and all Research Partner's Personnel as if they were the activities, omissions, or defaults of Research Partner.
 - (a) Research Partner may not subcontract any part of its obligations under the Agreement except as agreed in writing by Shell. Research Partner will ensure that subcontracts are in all material respects consistent with the terms and conditions of the Agreement, including the terms and conditions of Clause 8, in particular by extending the obligations under Clause 8.2 and 8.5 to include those Results obtained by Subcontractor and under Clause 8.3 to include Subcontractor's Intellectual Property Rights.
 - (b) Research Partner agrees to indemnify Shell and its Affiliates for liabilities arising from Research Partner's use of Subcontractors in the performance of the Agreement.

13. TERMINATION

- 13.1 Either Party may terminate this Agreement by giving notice to the other Party if the other Party commits a material breach of any term of this Agreement, whether or not such breach would otherwise qualify as a repudiatory breach at common law and which is either incapable of remedy, or, if capable of remedy is not remedied within thirty (30) days of service of notice by the Party not in breach requiring remedy.
- 13.2 Shell may terminate the Study with immediate effect by written notice in the event that:
 - (a) the Supervisor and/or Research Associate cease to be involved in the Study and the Research Partner is unable to find an alternative person(s) acceptable to Shell to supervise and/or carry out the Study, as the case may be;
 - (b) following consultation with the Research Partner Shell is of the opinion, that insufficient progress has been made towards the aims of the Study;
 - (c) the direction of the Study has changed significantly from that originally contemplated by Shell such that Shell is no longer interested in funding the Study; or
 - (d) the Research Partner or any of its personnel, employees or contractors, when performing work in connection with this Agreement;

- (A) commits any or causes Shell or any of its Related Parties to be in breach of applicable Anti-Bribery Laws;
 - (B) breaches Clause 14.5 of this Agreement;
 - (C) commits any or causes Shell or any of its Related Parties to be in breach of applicable competition laws; or
 - (D) commits a material breach of the Laws not mentioned in paragraphs (A) and (C) of this Clause; or
- (ii) any conflict of interest arises between the Research Partner or any of its Related Parties and Shell or any of its Related Parties, unless accepted in writing by Shell.
- 13.3 Shell may terminate the Agreement or reduce Study for convenience at its own discretion with thirty (30) days prior written notice. In the event of early termination, research partner shall be paid for all work performed and related expenses incurred, including any non-cancelable commitments, in accordance with this Agreement until the date of termination.
- 13.4 Provided that Shell satisfies its obligations under Clause 5 that are outstanding at the date of termination, Shell shall have no further obligations toward the Research Partner with respect to the Study after such termination.

14. COMPLIANCE WITH ANTI-BRIBERY LAWS

- 14.1 The Research Partner represents and warrants that, in connection with this Agreement or the business resulting therefrom:
- (a) it is knowledgeable about Anti-Bribery Laws applicable to the performance of this Agreement and will comply with all such laws;
 - (b) neither it nor a Related Party have made, offered or authorised or will make, offer or authorise any payment, gift, promise or other advantage, whether directly or through any other person or entity, to or for the use or benefit of any Government Official or any person where such payment, gift, promise or other advantage would (i) comprise a facilitation payment; and/or (ii) violate the Anti-Bribery Laws;
- 14.2 The Research Partner undertakes to immediately notify Shell if in connection with this Agreement or the business resulting therefrom it receives or becomes aware of any request from a Government Official or any person for any payment, gift, promise or other advantage of the type mentioned in Clause 14.1(b).
- 14.3 Shell confirms that its appointment of the Research Partner was expressly made on the basis that Anti-Bribery Laws and the Business Principles would not be violated. The Research Partner acknowledges that the contents of this Agreement may be disclosed by Shell to third parties for the purposes of demonstrating compliance with this Clause.
- 14.4 The Research Partner represents and warrants that neither it nor any of its Related Parties is a Government Official or other person who could assert illegal influence on behalf of Shell or its Affiliates. If any of the foregoing becomes a Government Official, the Research Partner shall promptly notify Shell.
- 14.5 The Research Partner shall indemnify, defend, and hold harmless Shell and its Related Parties from and against any and all losses, damages, claims, expenses, fines and penalties arising out of the Research Partner's representations in this Clause 14 being untrue or arising out of the Research Partner's breach of any of its warranties or undertakings in this Clause 14.

15. LIABILITIES AND INDEMNITIES

- (a) Liability for loss of and damage to property and for personal injury, death, or disease to any person, arising in connection with the Agreement, will be determined in accordance with applicable law.
- (b) Neither party will be liable to the other for that other party's own consequential loss, or any punitive or exemplary damages that might be awarded in that party's favour, regardless of negligence or other fault.
- (c) Neither party excludes or limits its liabilities to the extent they may not be excluded under applicable law.

16. INSURANCE

Prior to commencement of performance, Research Partner will arrange any insurance required by applicable law, and maintain such insurance in effect throughout the duration of the Agreement. Satisfaction of the obligation to procure insurance and perform other actions in connection with this Article will not relieve Research Partner of any other obligations or liabilities.

17. BUSINESS PRINCIPLES/CODE OF CONDUCT

17.1 The Research Partner acknowledges that:

- (a) it has received a copy of the Shell General Business Principles ("Business Principles") (or alternatively taken note of the Shell General Business Principles at www.shell.com/sgbp);
- (b) it has received a copy of the Shell Code of Conduct (or alternatively has taken note of the Shell Code of Conduct at http://www.shell.com/home/content/aboutshell/who_we_are/our_values/code_of_conduct/);
- (c) it has been made aware of the Shell Global Helpline at http://www.shell.com/home/content/aboutshell/who_we_are/our_values/compliance_helpline/.
- (d) it has received the Shell Supplier Principles (or alternatively taken note of the Shell Supplier Principles at <http://www.shell.com/suppliers>)

17.2 The Research Partner agrees that it and its Related Parties shall adhere to the principles contained in the Shell General Business Principles (or where The Research Partner has adopted equivalent principles, to those equivalent principles) in all its dealings with, for or on behalf of Shell in connection with this Agreement and the business resulting therefrom. In the event that the Research Partner or any of its Related Parties supply staff that work on behalf of Shell or represent Shell, the Research Partner commits that such staff will behave in a manner that is consistent with the Shell Code of Conduct. The Research Partner shall notify Shell immediately if it becomes aware of any behaviour by Shell staff, the Research Partner or its Related Parties which is, or may be, inconsistent with the Shell General Business Principles, the Shell Code of Conduct or, where the Research Partner has adopted equivalent principles, their equivalent.

17.3 At Shell's request, the Research Partner will provide information to Shell as required to complete and fully respond to Shell's usual supplier questionnaires and due diligence to confirm compliance by Research Partner with Business Principles. As part of Shell's due diligence, Research Partner will grant Shell or its representatives reasonable access to the Research Partner's facilities and sites.

18. FINANCIAL AND PERFORMANCE AUDIT

- (a) Shell will have the right to audit: (i) invoiced charges and proper invoicing; (ii) other books and records; and (iii) the performance of any other of Research Partners' obligations under the Agreement, including compliance with Anti-Bribery Laws, where capable of being verified by audit. For the duration of this right see the terms under c.

- (b) Based on the findings of the audit the parties will settle any amounts charged incorrectly within forty five (45) days of any audit finding; and Research Partner will provide any Study, or refund, repair, replace, or re-perform any Study where the requirement to do so is identified by any audit within forty five (45) days of any audit finding.
- (c) Research Partner will keep books and records available for audit for the longer of the following periods: (i) five (5) years following termination of the Agreement or any longer period as required by applicable laws; or (ii) two (2) years after the period expires on any obligation of Research Partner to refund, repair, replace, or re-perform any Study (including correction of defects). Research Partner will keep books and records relating to compliance with Anti-Bribery Laws available for audit for the period prescribed in the Agreement for retention of such records.

19. HSSE & EXPORT CONTROLS

19.1 In performing all work in connection with the Agreement, Parties and Parties Personnel will strictly comply with all applicable laws. Whenever Parties are on a Worksite they shall behave in a manner which is consistent the requirements for the management of health, safety, security, and environmental protection, as well as any rules, procedures or codes of practice in force at the relevant Worksite. Research Partner shall at all times be aware of the Goal Zero principle and Shell's Life Saving Rules. Research Partner confirms having received a copy of Shell's Life Saving Rules (or alternatively, has taken notice of the Life Saving Rules at http://www.shell.com/home/content/environment_society/safety/culture/).

- 19.2 (a) *Trade Control Laws.* Research Partner acknowledges that it is familiar with and will comply with all applicable Trade Control Laws. Without prejudice to the foregoing, Research Partner will provide Shell, in writing, with the relevant Export Control Classification Number (ECCN) and applicable jurisdiction(s) for any dual-use or military items (i.e. goods, software, or technology). Without limiting the foregoing, Research Partner will ensure that Shell Information is used in accordance with applicable Trade Control Laws.
- (b) *Export/Import Licences.* Unless otherwise agreed between the parties in writing, Research Partner will be responsible for obtaining all necessary import and export licences and/or any other customs licence as required by applicable laws for the Results. Where such licenses or authorizations are obtained, Research Partner will provide Shell written notice of all applicable conditions, including but not limited to those restricting the further export, use or release of the Results.
- (c) *Restricted Jurisdictions and Restricted Parties.* Research Partner will ensure that (i) except with the prior written consent of Shell, Shell Information is not exported, provided or made available to any Restricted Jurisdiction or Restricted Parties (ii) subcontractors are not Restricted Parties and (iii) except with the prior written consent of Shell, Research Partner Personnel engaged in the Study are not Restricted Parties or nationals of a Restricted Jurisdiction. Without limiting the foregoing, Research Partner will at relevant times screen subcontractors and Research Partner Personnel against governmental lists to ensure none are a Restricted Party.

20. PERSONAL DATA PROTECTION

Where Research Partner is required to process Personal Data on behalf of Shell to perform the Study, Research Partner agrees to comply, and ensure its Related Parties comply, with the relevant applicable laws. Any member of Research Partner and its Related Parties processing Personal Data must enter into a standard form data processing agreement as advised by Shell.

21. COMPLIANCE WITH REACH REGULATIONS

- (a) In all cases where applicable due to Study provided, Research Partner agrees to comply with Regulation (EC) No. 1907/2006 ("REACH"), and Research Partner warrants that:
 - (i) any substances, within the meaning of the REACH regulation, in Study have been validly pre-registered or immediately registered (as applicable) in accordance with REACH; (and Research Partner will confirm and provide evidence of compliance in writing to Shell prior to dispatch of those items);
 - (ii) where substances in Study have been pre-registered, Research Partner will take all necessary steps to ensure that those substances are validly registered in accordance with REACH according to the deadlines set out in REACH;
 - (iii) any registration will cover Shell's uses and applications of the substances (or those of Shell's customers) where these have been notified to Research Partner (or to Research Partner's "only representative" if appointed and notified to Shell) no later than three months before the relevant registration deadline; and
 - (iv) any registration will be kept up-to-date (including any relevant amendment to uses).
- (b) Research Partner will immediately notify Shell in writing if any substance in Study may or has become subject to an authorisation or restriction under REACH or where any circumstance has arisen that would call into question whether any substance in Study is adequately registered.
- (c) Research Partner will provide Shell with a copy of the current safety data sheets for Study in the format and containing the information required by REACH. Research Partner will send a copy of the safety data sheet in the language and to the address or contact as advised by Shell.

22. TAXATION

- 22.1 The Research Partner will be responsible for and indemnify Shell from all taxes, levies, social securities and other charges and duties imposed in connection with the provision of the Services and the supply of goods and intangible property (referred to as "Tax"), except for value added tax in countries of the European Union or an equivalent sales tax which is due in respect of the supply from the Research Partner to Shell (the above mentioned value added tax and equivalent sales tax are collectively referred to as "Indirect Tax").
- 22.2 To the extent that the provision of the work and the Results and intangible property are subject to Indirect Tax which is due as described above, the amount of such tax will be added to the fee on the invoice. Shell specifically does not accept responsibility for any Indirect Tax that relates to purchases by the Research Partner or the Research Partner's suppliers. Where legally possible, the Research Partner will apply a tax exemption, 0% rate or any other tax facility applicable in the relevant country. In the case Shell has to pay a withholding tax to the tax authorities under the applicable tax regime(s), Shell shall pay to the Research Partner the amount of the invoice after deduction of such tax.
- 22.3 In the event that a refund opportunity arises with respect to any Tax paid by one party as a result of the transactions governed by this Agreement, both Parties shall reasonably work together to pursue such refund. If one party receives a refund or a credit for any Tax paid by the other party, then the party receiving the refund or credit agrees to refund to that other party the full amount of such refund or credit.
- 22.4 In the event that the Research Partner is considered to have a permanent establishment in any country occasioned by the supply of goods or delivery of services under the Agreement, the Research Partner shall be solely liable for (a) any liability for taxes and (b) any and all other costs incurred by the Research Partner due to such permanent establishment.
- 22.5 The Research Partner and Research Partner Personnel render the services under this Agreement as independent Party(ies) and is(are) not authorized to act as the agent or representative of Shell or to represent that it or they are entitled so to act. The Research Partner and Shell agree that no employment relationship shall exist between Shell or any Affiliates and Research Partner Personnel. The Research Partner will maintain complete control over and have full responsibility for the performance of its personnel, agents, consultants and subcontractors. Shell reserves no right to direct, supervise or control the operations, personnel, agents, consultants or subcontractors of the Research Partner. Accordingly the Research Partner and Shell agree as follows:

- (a) The Research Partner shall be responsible for ensuring that all wages, fees, contributions and all social security and other contributions including for the avoidance of doubt National insurance contributions, charges and taxes required to be paid by the Research Partner in respect of Research Partner Personnel are paid, together with any payments due or in respect of any Generally Embargoed Country (GEC) personnel required by law; and
 - (b) The Research Partner shall ensure that all appropriate deductions are made from the wages of the Research Partner's personnel in respect of taxes, employees social security and other contributions including for the avoidance of doubt national insurance contributions.
- 22.6 The Research Partner is fully responsible for its personnel and the Research Partner vis-à-vis Shell assumes full and exclusive liability for payments of claims for salaries, benefits, indemnities and other demands related to the employment, that are made by Research Partner Personnel, or their dependants or successors. Neither the Research Partner nor Research Partner Personnel shall be deemed to be either expressly or implicitly employees of Shell. Should it ever be determined that the Research Partner or Research Partner Personnel acted under this Agreement as an employee or co-employee of Shell and/or its parent(s), affiliates and subsidiary companies, then to the maximum extent permitted by law, the Research Partner shall defend, indemnify and hold harmless Shell, its parent(s), affiliates, and subsidiary companies against (i) any loss, damage, claim, suit, liability, judgment and expense (including, but not limited to, attorneys' fees and other costs of litigation), (ii) any fines, penalties, or assessments, arising out of any such determination, and (iii) any claim of coverage or eligibility under any of the compensation arrangements or benefit plans of Shell and/or its parent(s), affiliates and subsidiary companies.

23. ASSIGNMENT AND SUB-CONTRACTING

- 23.1 The Research Partner shall not assign all or any of its rights or obligations under this Agreement.
- 23.2 Shell may at any time assign all or any part of the benefit of, or its rights or benefits and/or obligations under this Agreement. Shell shall be free to arrange for any of its obligations and/or rights under this Agreement to be performed or exercised respectively by one or more Affiliates of Shell and/or other third parties.

24. AMENDMENTS AND VARIATIONS

This Agreement may not be amended or modified orally and no amendment or modification shall be effective unless it is in writing and signed by the authorised representatives of each of the Parties.

25. LAW AND JURISDICTION

- 25.1 This Agreement and any dispute or claim arising out of or in connection with it or its subject matter or formation (including non-contractual disputes or claims) shall be governed by and construed in accordance with the laws of The Netherlands with the exception of its private international law. The applicability of the 1980 Vienna Sales Convention (CISG) is excluded.
- 25.2 The parties irrevocably agree that the courts of The Hague, The Netherlands shall have exclusive jurisdiction to settle any dispute or claim that arises out of or in connection with this Agreement or its subject matter or formation (including non-contractual disputes or claims).

26. MISCELLANEOUS

- 26.2 Failure or delay by Parties in enforcing or partially enforcing any provision of the Agreement shall not be construed as a waiver of any of its rights under the Agreement.
- 26.3 Any waiver by Shell of any breach of, or any default under, any provision of the Agreement by Research Partner shall not be deemed a waiver of any subsequent breach or default and shall in no way affect the other terms of the Agreement.
- 26.4 The rights and remedies provided by the Agreement are cumulative and not exclusive of any rights or remedies provided in law, equity, or otherwise and shall extend to Shell's successors and assigns.

- 26.5 This Agreement may be executed and delivered by the parties in counterparts (each of which shall be considered for all purposes an original) and by facsimile and when a counterpart has been executed and delivered by each of the parties, by facsimile or otherwise, all such counterparts and facsimiles shall together constitute one agreement.
- 26.6 The covenants, conditions and provisions contained in the Agreement which the parties intend to survive, including confidentiality obligations, intellectual property rights and liabilities, audit rights, warranties, applicable law, dispute resolution, and indemnities, survive termination and expiry of the Agreement for the benefit of the party or parties to whom they are given. In addition, the expiry or termination of the Agreement does not discharge or release either party from any liability or obligation accrued at the time of such expiry or termination or continuing beyond or arising out of such expiry or termination.
- 26.7 This Agreement constitutes the entire agreement between the parties hereto and supersedes all prior negotiations, representations or agreements related to the subject matter hereof, either written or oral. No amendments to the Agreement, nor any contrary or additional conditions specified by Research Partner in any document provided by Research Partner, shall be effective unless evidenced in writing and signed by the parties hereto.
- 26.8 In the case of any conflict between the terms of the Appendices and this Agreement, the terms of this Agreement shall prevail.
- 26.9 The concept of severability of clauses applies.

AS WITNESS WHEREOF, the Parties have caused this Agreement to be executed in duplicate original at the places and on the dates specified below.

For and on behalf of [REDACTED] 5.1.2e
Shell Global Solutions International B.V.

[REDACTED] 5.1.2e
[REDACTED] 5.1.2e

[REDACTED] 5.1.2e
Title: [REDACTED] 5.1.2e

Place: Amsterdam

Date: 14/12/10

For and on behalf of
LEIDEN UNIVERSITY

Signature:

5.1.2e

By:

Title:

Place:

Leiden.....

Date:

December 13, 2010

APPENDIX I

THE STUDY

Quantum chemistry on a quantum computer

Principal investigators:

- 5.1.2e physics department, Leiden University (5.1.2e)
- 5.1.2e chemistry department, Leiden University
- 5.1.2e Shell Research

Abstract:

Quantum chemistry in its various forms is one of the largest consumers of supercomputer time worldwide and at Shell. Due to the computational intensity of solving Schrödinger's equation for the electrons exactly, approximate solutions are the only practical approach. A quantum computer with 100 logical qubits can potentially already solve problems involving chemical systems of interest faster and more accurately than classical computers. One can finally imagine the "correct" calculation of reaction pathways, and for revolutionary applications ranging from environmentally friendly fertilizers to novel bio-pharmaceuticals or catalysts for the conversion of carbon dioxide to fuels. Quantum chemistry is widely considered one of the first tangible contributions of quantum computers to society. The Netherlands is a leader in the development of quantum computing hardware, but quantum software development has remained largely unexplored. Here we propose a focused pilot study to identify promising directions for research and development in quantum computational chemistry in an interdisciplinary team involving physicists and chemists from academia and industry. Comparisons with existing state-of-the-art methods on classical computers are an integral part of this study, thus addressing the important issue of quantum speedup.

Background:

The concept of a quantum computer is quickly becoming reality. Hardware with 50 qubits is accessible in the cloud. This is not yet sufficient to overtake a conventional (classical) computer but enough to meaningfully try out small-scale applications. Quantum chemistry is one such application and of great interest Shell. A recent NSF study in the US has made an inventory of "Quantum Information and Computation for Chemistry".

In The Netherlands the National Science Agenda has funded a small pilot study to explore "quantum chemistry on a quantum computer". The four authors of this proposal are carrying out this study in collaboration with the hardware developers at QuTech in Delft. In this document we describe a proposal for a joint program with Shell Technology.

Expected impact:

By the end of this five-year project we will have simulated quantum computations of small to medium-sized (10-50 electronic states and qubits) molecules in the absence of error, and small (2-15 electronic states and qubits) molecules in the presence of noisy quantum hardware. This will allow us to make connection to current and near-future experimental quantum computations of small molecules, and extrapolate this to the requirements for simulating properties of large (100 electronic states and qubits) molecules that lie beyond the ability of classical computational chemistry techniques. This will be complemented by performance comparisons with state-of-the-art classical computation techniques such as density functional theory (DFT), quantum Monte Carlo (QMC), coupled cluster (CC), and density matrix renormalization group. As part of this, we will pave the way for the quantum simulation of extended organic molecules and systems with transition metal elements by implementing and optimizing current techniques for quantum simulation. We will further develop hybrid quantum-classical

computer techniques for embedded systems, external potentials, and excited state dynamics for photochemistry. We will then prepare for larger quantum computers that could become available in the next 5 to 10 years by identifying particularly valuable targets for simulation and by designing the fault-tolerant circuits that will establish the usefulness of a quantum computer for computational chemistry.

Workplan:

The project consists of two distinct streams, a 'top-down' approach and a 'bottom-up' approach.

The initial stages of the 'bottom-up' approach will consist of optimizing quantum phase estimation and variational circuits for small quantum simulations of light diatomic and other small molecules to be performed on experimental hardware in a partner project on superconducting qubits in Delft¹. Attention will be paid to (1) the matching of results to previously reported experimental results and classical simulations (it being within the grasp of classical computation techniques); (2) the optimization of circuits for the experimental systems they are being performed on, (3) the development and implementation of error mitigation techniques for noisy near-term quantum computers, and (4) ensuring that all techniques used are scalable to larger and fault-tolerant systems. From here, we will progress to the study of larger (~50) qubit systems on classical simulators. As part of this, we will develop methods for approximating errors in simulated quantum computers when realistic error models are no longer feasible computationally. An open question, which we will attempt to answer during this time, is whether this quantum fault-tolerance overhead may be reduced below that of the surface code. This would allow an intermediate step between the current small-scale experimental attempts and truly large-scale future quantum computers with a projected number of 107 qubits.

The 'top-down' approach will begin by using existing software (for example OpenFermion) to develop and cost quantum circuits for standard reference problems in quantum chemistry such as ordering the spin states in Iron porphyrin and determining the ground state potential energy curves of He₂, Be₂, Cr₂ and Fe₂. This will allow a comparison to state-of-the-art quantum chemistry techniques for strongly correlated systems, such as quantum Monte Carlo, multi-reference coupled cluster, and density matrix renormalization group. After this, we will begin compiling a list of potential simulation targets for a future quantum computer, focusing on both their value as simulation targets and their cost for a future quantum computer. Alongside this, we will work to develop hybrid quantum-classical algorithms (among others, based on the widely-used ADF software) to allow for the embedding of quantum simulations in larger systems, and to study excited-state and dynamic properties of molecules such as photo-induced electron transfer. A key part of this will be predicting the technical requirements for a future quantum computer to break the 'usefulness threshold' (and at what point this might be achieved), and generating a list of simulations to be performed on this first generation of commercial quantum computers.

Each individual project described in the above timeline represents a necessary step towards the usage of future quantum computers for quantum chemistry and molecular dynamics research. These developments are especially necessary to inform future experimental and theoretical quantum computing research directions. Sequential projects within individual streams will build on former projects, however the two streams are separate enough that one may still progress while the others are halted (in case of experimental or computational difficulties).

Summary of projects:

1. Optimizing quantum circuits for near-term and first-commercial quantum chemistry applications.
2. Comparing quantum computing performance to state-of-the-art computational chemistry and integrating quantum computing algorithms with quantum chemistry packages.

¹ At the present stage we are implementing quantum algorithms on non-topological superconducting qubits (the Delft roadmap plans for 50 qubit devices in the cloud by the end of 2020). The topological qubits being developed by Delft in collaboration with Microsoft are not yet at this stage but our algorithms will be platform-agnostic and will be ready to be deployed on topological hardware when it becomes available.

3. Quantum algorithms beyond the static ground state; simulating excited states, molecular dynamics, and embedded systems.
4. Designing workflows targeting first quantum chemistry problems on a quantum computer.

Interacting and aligning with current Shell research:

Quantum chemistry is a part of Shell's Computational chemistry program executing mostly in Bangalore. The Shell Bangalore team both conducts fundamental R&D and assists the Shell catalysis and New Energies businesses developing superior products. DFT is the dominant quantum method, and computational chemistry uses 5-10% of Shell's large HPC resources. The systems of interest are often highly correlated organic or metallic in nature, and all DFT solutions incur severe unknown approximation errors. Shell R&D will assist the present project with identifying target problems which are of sufficient value to industry to justify costly quantum simulation. In return, we can advise Shell chemists on the potential and timeframe for quantum computers to assist in solving relevant research problems, how such calculations would be performed in practice, and provide training to Shell in preparing for the use of quantum computers. As ancillary benefit, Shell will learn through this project what problems can be solved with "beyond-DFT" methods" such as FCIQMC, CC and density matrix based approaches, and how to even think about "exact" solutions. Such methods are currently not in use in Shell due to overwhelming computational demand.

APPENDIX II

PAYMENT SCHEDULE

In full and final settlement for the performance of the Study, the production and issue of the Results, the granting of Rights, and for fulfilling and/or complying with all other terms and conditions of the agreement Shell shall pay to the Research Partner the total amount of 5.12b.5.1.2f (Excluding VAT and Excluding Travel Expenses)

	Year 1	Year 2	Year 3	Year 4	Year 5	Total
Research Associate	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f
Postdoc	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f	5.12b.5.1.2f

This amount shall be paid in six 5 installments as follows:

First installment of EURO 5.12b.5.1.2f	due date: after contract signature
Second installment of EURO 5.12b.5.1.2f	due date: December 2019
Third installment of EURO 5.12b.5.1.2f	due date: December 2020
Fourth installment of EURO 5.12b.5.1.2f	due date: December 2021
Last installment of EURO 5.12b.5.1.2f	due date: at the end of the Study upon receipt of the final report and deliverables.

To the extent authorized, Shell shall reimburse all out-of-pocket travel and lodging expenses as part of the Study for Research Partner at actual cost (including, but not limited to, hotel, airfares and car rentals collectively "Travel Expenses") provided that such Travel Expenses are documented with receipts and are attached to the invoice. Travel shall be at normal coach/economy class fares; overnight lodging shall be at rates comparable to standard economy room rates. Research Partner shall arrange alternatives to hotel expenses (e.g. apartment rentals, corporate housing, etc.) and local transportation (e.g. sharing of rental cars, etc.) to minimize lodging expenses where cost effective.

Travel expenses shall be invoiced together with each installment.

Travel expenses estimated at 5.12b.5.1.2f Euro in total.

APPENDIX III

MILESTONES AND DELIVERABLES FOR SHELL/LEIDEN COLLABORATION

1. Year 1 objectives/milestones:

- Determine quantities of interest for quantum chemistry can be easily calculated on a quantum computer.
- Develop fair metrics for comparing quantum and classical computers for quantum chemistry.
- Learn to calculate cost of algorithms on future quantum computers (e.g. T-gate counting).

2. Year 1 deliverables:

- Paper on calculating gradients on quantum computer.
- Paper on new methods for state preparation on a quantum computer.
- Interface between Openfermion and Dirac code
- Code to convert quantum computing output to chemistry data added to Openfermion.

3. Year 2 objectives/milestones:

- Compile list of 'good' problems for a quantum computer (i.e. the easiest problems for a quantum computer to compete with a classical computer in solving).
- Compare quantum computing power to some classical methods on few target problems.
- Calculate how much error mitigation can improve NISQ-era quantum computers.

4. Year 2 deliverables:

- Paper on embedding quantum computation in studies of larger systems.
- Paper comparing simulated quantum computing to classical computing.
- Code to embed quantum computing subroutines in larger classical calculations.
- Extensions and additions to openfermion routines for quantum circuitry.

5. Year 3 objectives/milestones:

- Determine/predict whether quantum computers will achieve useful results in quantum chemistry without error correction.
- Extend testing of simulated quantum computing against classical methods to more examples/methods.
- Extend study of quantum computing ability for excited states and dynamics.

6. Year 3 deliverables:

- Paper on calculating excited states/dynamics on a quantum computer.
- Paper on limits of error mitigation for near-term quantum computers.
- Code to calculate excited states/dynamics on a quantum computer.
- Extensions and additions to openfermion routines for quantum circuitry.