

ONETEP Software Academic User Licence Agreement

1. Definitions

“USER” means(name)

“INSTITUTION” means.....

.....(title and address of institution)

“Effective Date” means.....(date of signing)

“CE” means Cambridge Enterprise Limited, whose registered office is at The Old Schools, Trinity Lane, Cambridge CB2 1TN.

ONETEP Developers’ Group (“ODG”) means the informal group that created and developed the ONETEP Software currently consisting of the following members, Peter Haynes, Chris-Kriton Skylaris, Arash Mostofi, Nick Hine, Jacek Dziedzic and Michael Payne.

“Software” means the most recent, stable version of the ONETEP distribution on the Effective Date.

2. Licence

2.1 This licence agreement (“Agreement”) shall be effective from the Effective Date written above and is between CE and the USER. The Agreement requires that the USER has a permanent or tenured contract (“a Permanent-post Academic”), not a fixed term or temporary contract, or an independently funded research fellowship, at the INSTITUTION. If the USER ceases to be a Permanent-post Academic or an independently funded research fellow at the INSTITUTION, the Agreement will terminate immediately, subject to the provisions in Clause 2.4.

2.2 Under this Agreement CE agrees that CE will provide and the USER will accept a non-exclusive and non-transferable licence for the use of the Software on the terms and conditions specified in this Agreement. The licence provided by this Agreement extends to members of the USER’s academic research group (“Group”), provided they are students or employees of the INSTITUTION. If any member of the Group ceases to be a student or employee of the INSTITUTION their licence to the Software will terminate immediately.

2.3 This Agreement allows the USER and Group to use the Software for their academic use and research needs only. Use of the Software, or any code which is a modification of, enhancement to, derived from or based upon the Software, for

industrially funded research or for providing services to a non-academic third party is expressly prohibited, except in the case of a member of the Group carrying out research that is funded by a CASE studentship. The licence allows the Software to be used by the USER and the Group for collaboration with other research groups within the INSTITUTION and with research groups within other academic institutions.

2.4 In the event that the USER ceases to be a Permanent-post Academic or an independently funded research fellow at the INSTITUTION, CE will at their discretion and in consultation with the ODG offer individual members of the Group at their request written permission to continue using the Software under the licence provided in this Agreement. The continuation of the licence will be limited to the individual and the work specified in the written permission provided by CE. Upon completion or cessation of the specified work, this licence will terminate immediately.

2.5 This Agreement allows the Software to be used on an unlimited number of processors with no constraint on where these processors are located.

3. Publication

3.1 All published work; including journal and conference papers and theses; produced in part using the Software must cite the paper "Introducing ONETEP: Linear-scaling density functional simulations on parallel computers" C.-K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne. *J. Chem. Phys.* **122**, 084119 (2005)" along with any other relevant ONETEP references. The USER must be listed as the author or a co-author on this work.

4. Code Provision and Software Maintenance

4.1 Upon receipt of a completed version of this Agreement, CE will procure that the ODG will send a copy of the Software to the USER. This will contain the latest stable ONETEP distribution.

4.2 The Software is provided "As Is" and except as expressly provided in this Agreement no warranty, condition, undertaking or term, express or implied, statutory or otherwise, as to the condition, performance, satisfactory quality or fitness for purpose of the Software is given or assumed by CE or the ODG and all such warranties, conditions, undertakings and terms are hereby excluded.

5. Intellectual Property

5.1 The Software is the subject of copyright. Unauthorised copying of the Software is expressly forbidden. CE retains all the rights in and title to the Software. The USER may not sublicense, distribute or copy (except for archival purposes) the Software or enhancements thereto.

5.2 This Agreement allows the USER or Group to produce additional functionality or code development for the Software ("Additional Functionality"). If this occurs, the USER shall inform CE promptly of such Additional Functionality. The USER shall and hereby does agree to grant a worldwide, royalty free licence with right to grant sub-licences of such Additional Functionality to CE who shall have unrestricted rights to license such Additional Functionality solely for academic purposes. The USER shall give CE a right of first refusal to obtain an exclusive worldwide licence, including the right to sub-licence, to distribute such Additional Functionality. The USER shall negotiate in good faith the terms and conditions of the licence with CE. Aside from the foregoing, the USER and Group shall have no right to use (other than for their personal non-commercial use), market, sell, distribute or commercially exploit in any way any Additional Functionality for use with the Software, and may not refer to the Software in connection with any commercial use of Additional Functionality in any other software product without the prior express permission of CE.

5.3 The USER undertakes to treat as confidential and keep secret (i) the Software program code, (ii) the Software specification and (iii) all information which is otherwise clearly identified as confidential. The obligations in this clause shall remain in full force and effect indefinitely, notwithstanding any termination of this Agreement.

6. Termination

6.1 This Agreement will terminate automatically on notice from CE if the USER fails to comply with any provision of this Agreement. Upon termination the USER shall immediately destroy all copies of the Software. No refunds or credits will be due.

6.2 The licence to Additional Functionality granted to CE, provided for in clause 5.2 of this Agreement, shall survive termination of this Agreement indefinitely.

7. Miscellaneous

7.1 All notices required hereunder shall be in writing and sent by recorded delivery, or other overnight courier to the addresses written above, or such other address as noticed to the parties.

7.2 This Agreement and any matters relating to it shall be governed and construed in accordance with the laws of England and Wales and CE and the USER hereby irrevocably submit to the exclusive jurisdiction of the English Courts.

Signed by the USER:

Signature _____ Date _____

Print name _____

Signed for and on behalf of CE:

Signature _____ Date _____

Print name _____

Position _____

Contact Details

To allow us to contact you, please provide us with your e-mail and work address. Only one copy of this page needs to be submitted.

User's name: _____

E-mail: _____

Work Address: _____
