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ARTICLE 1 DEFINITIONS

Agreement: the agreement between You and SCM for the use of the Software. Unless explicitly specified otherwise in writing, the Agreement consists of the Offer letter and these License Terms.

License Terms: these license terms as part of the Agreement, including all exhibits thereto.

IP-rights: any and all intellectual property rights, including but not limited to copyrights, neighbouring rights, registered and unregistered (trade)marks, tradename rights, patents and sui generis database rights, as well as know how and trade secrets contained in or relating to SCM and the Software.

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Research group: the research group as mentioned in the Offer letter, if applicable.

Software: the software programs distributed by SCM including, without limitation, object code, components, designs, specs, listings, algorithms, diagrams, graphs, data, calculations, adjustments, any revisions, updates and/or upgrades thereto, including the Data files defined below. Software will include Documentation and Third Party Software.

Data files: all data files in the distribution, including but not limited to the databases or parameters or geometrical structures of molecules or structures that are incorporated in the Software or delivered with the Software in encrypted or unencrypted form, including but not limited to DFTB parameters and ReaxFF parameters, including data related to Third Party Software.

Documentation: any online or otherwise enclosed documentation regarding the Software, provided by SCM.

Offer letter: written statement (usually by email) by SCM in response to a request for a price quotation sent by You. The Offer letter may contain specific license terms, restrictions, price specifications and payment terms.

Third Party Software: software, which is owned and controlled by third parties and is embedded in and/or distributed together with the SCM Software, including, but not limited to open source software.

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You: the natural person or legal entity that has entered into an Agreement with SCM.

ARTICLE 2 APPLICABILITY

2.1 These License Terms are applicable to all use of the Software by You, whether or not You have entered into an Agreement with SCM for the use of the Software.

2.2 An Offer letter will be deemed to have been accepted by You and an Agreement concluded either by means of a written confirmation of the Offer letter or if payment of the price as specified in the Offer letter has taken place. In the latter case the content of the Offer letter and these License Terms will be deemed to have been agreed to.

2.3 In case of any inconsistency between the Offer letter and the License Terms, the Offer letter will prevail.

2.4 The applicability of Your general terms and conditions is expressly excluded.

2.5 Any deviations from the License Terms are only valid if agreed upon in writing between You and the statutory director of SCM. These deviations will be incorporated in an addendum to the Agreement.

2.6 You hereby represent and warrant that You are authorized to bind the entity identified in the Offer letter to these License Terms.

2.7 The Agreement does not constitute a purchase agreement under applicable law.

2.8 These License Terms may be amended by SCM in case of substantial company interests and will notify you of such changes. If You do not agree to the changes, the only option available to You is to end Your use of the Software and to terminate the Agreement in accordance with article 10.

ARTICLE 3 DEMO LICENSE

3.1 If You are using the Software as part of a free evaluation period, the stipulations of this article shall apply, in addition to the other articles of the License Terms. Article 9 and 10 shall not apply. You will not receive a formal Offer letter for the free evaluation period. Any restrictions or conditions set out in an email or in the license file will apply to Your use of the Software.

3.2 Unless otherwise agreed upon in writing by SCM, the free evaluation period shall be 1 month from the start date of the trial (the moment you receive download access to the software).

3.3 SCM may immediately terminate your trial period in writing at any time, without cause and without becoming liable to You.

3.4 After termination or expiry of the trial period You must destroy all copies of the Software and Documentation in your possession.

3.5 In addition to the restrictions in Article 6, during the free evaluation, the software may be used only for evaluation purposes and not for research. In particular, the results obtained with an evaluation license may not be used for a scientific publication.

ARTICLE 4 GRANT OF LICENSE

4.1 Subject to the terms and conditions of the Agreement and the payment of all applicable license fees, SCM grants to You a limited, non-exclusive and non-transferable license to install and use the Software for the purposes as set out in the Agreement and on the number of processor cores and for the user groups within Your Institute as specified in the Agreement.

4.2 You will ensure that SCM is at all times aware of the relevant information regarding the number of processor cores in the machines on which You wish to use Software.

4.3 You may make or store a maximum of 2 backup copies of the Software per version for archival purposes.

4.4 You are entitled to sublicense the right to use the Software as provided to you in the Agreement to user groups consistent with the purchased license type, subject to the maximum amount of cores as specified in the Offer letter. You guarantee that You will inform these users of the applicability of these License Terms and You acknowledge that You will be responsible and liable for their compliance with the Agreement and any use of the Software by the users.

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5.1 When You publish results obtained with the Software in (scientific) literature, You must include proper references, as specified in the Software itself and/or in the Documentation, such as the "Required Citations" document. Results obtained with the Software means any data, lists, specifications and calculations for which the Software was in any way used.

5.2 In any publication of results obtained with the Data files, You will indicate the name(s) of the Data files used in Your calculations, and You will make reference to those publications, in which the construction and tests of the used Data files are described. For every Data file the publication to cite is given in the documentation section

of the file. In a case of discrepancy the papers specified in the Data files are authoritative. References related to DFTB.org parameters may also be found on www.dftb.org.

ARTICLE 6 RESTRICTIONS

6.1 These License Terms grant You the right to use the Software for internal purposes only. Internal purposes are to be understood as the own, internal research purposes of the Institute specified in the Offer letter.

6.2 In case of an academic, government lab, academic computing center license, or other non-profit license You may use the Software exclusively for non-profit research purposes.

6.3. In case of an Academic Research group license, only members and students of the Research group specified in the Offer letter may use the software. In case of an Academic site (multiple academic group) license, only members and students of the specified site of the specified Academic Institute may use the software. Only degree-granting institutes are considered as being academic. In case of an academic computing center license, only users from academic (i.e. degree-granting) institutes may be given access to the software.

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- use the Software to aid (directly or indirectly) in the development or production of nuclear, chemical, biological or other weapons of mass destruction.

6.5 Except as specifically allowed in these License Terms, You may not retrieve or publish the entire databases incorporated in each Data file or retrieve or reuse, from a qualitative or quantitative point of view, a substantial part of its contents. Repeatedly and systematically retrieving or reusing parts of the Data files that are non-substantial from a qualitative or quantitative point of view, with the ultimate object of reconstructing the entire Data file or a substantial part thereof is also not allowed.

6.6 You understand and agree that additional restrictions may be specified in the Offer letter.

6.7 Any use of the Software by any third party, except as explicitly allowed in the Agreement, is strictly forbidden and constitutes a material breach of the Agreement.

6.8 Unless otherwise agreed upon, the usage rights are restricted to computers at one geographical site where your Institute is located.

ARTICLE 7 OWNERSHIP

7.1 You acknowledge and agree that the title to and ownership of the Software and the Data files and the IP-rights associated therewith are and remain the sole and exclusive property of SCM and its licensors. You do not purchase the Software but only obtain a license to use it for the agreed period of time and under the agreed

conditions and restrictions. You therefore have no right, title or interest in or to the Software and the IP-rights associated therewith, except as expressly set forth in these License Terms.

7.2 SCM or a representative appointed by SCM may, at any time during Your normal business hours and upon reasonable advance notice, conduct an audit at Your premises to ascertain whether Your use of the Software is in compliance with the provisions of the Agreement.

ARTICLE 8 DELIVERY

8.1 SCM distributes the Software in electronic form at SCM's website.

8.2 The Software and license keys for usage will be made available to You after the Agreement has been reached. A license file or any other security device that is provided by SCM, is provided to You for Your use of the Software, after you have provided SCM with up-to-date information regarding the number of processor cores in the machines on which you wish to use Software. You may not share or transfer the license file or other security device with or to any other user of the Software or any other third party (except those users within Your Institute entitled to use Your installation of Software under the License Terms).

8.3 The source code of the Software shall not be made available to You unless specifically agreed upon in the Offer letter.

ARTICLE 9 PAYMENTS; TAXES

9.1 The applicable license fees, payment terms, and specific license conditions (including for example the license term, number of processor cores, allowed users, licensed modules of Software) are set out in the Offer letter.

9.2 All payable amounts are net, exclusive of any Value Added Tax or other taxes or duties that may be imposed as a result of the transactions under these License Terms.

9.3 You shall pay each amount due within 30 days of invoice. If after the expiry of this period payment (in full) has not yet been received by SCM, You will immediately be in default without prior demand or notice of default being required. As from the time of default You will be liable for the statutory commercial interest, counting a part of a month as a full month, compounded from the due date.

9.4 If You despite demand or notice of default still fail to pay the claim, SCM may hand over the claim for collection. In that event all costs incurred by SCM in connection with overdue payments, such as legal costs and extra-judicial and judicial costs, including the costs of legal assistance, bailiffs and collection agencies, will be payable by You. The extra-judicial costs are fixed at no less than 10% of the invoiced amount subject to a minimum of €250 excluding VAT.

9.5 Complaints in relation to invoices and/or the Software will not suspend Your payment obligations.

9.6 SCM will be entitled to suspend the fulfilment of its obligations until such time as You have fully complied with all Your due obligations.

ARTICLE 10 TERM AND TERMINATION

10.1 The license will be effective for the period of time agreed upon in the Offer letter unless terminated sooner in accordance with the terms of these License Terms.

10.2 At any time Parties may negotiate an extension or renewal of the term. These License Terms will control all such extensions and renewals - even if established after a temporary discontinuation of the license - unless parties agree in writing upon a modification of the clauses.

10.3 If You infringe SCM's IP Rights, including but not limited to a breach of articles 4 and 6 of these License Terms, SCM reserves the right, with immediate effect and without becoming liable to pay compensation, to terminate the Agreement in writing, without prejudice to SCM's right to take further legal action and/or its entitlement to compensation.

10.4 Termination of the Agreement based on an attributable breach is only permitted in case of a material breach and after notice of default that gives as much detail as possible, and in which a reasonable term is set in which the breach can be remedied, unless these License Terms provide otherwise.

10.5 In the event of termination of the Agreement, no reversal will take place of that which SCM has already delivered and/or performed. Amounts invoiced by SCM before the termination in connection with that which SCM has already properly performed or delivered in the implementation of the Agreement will continue to be owed with due observance of the provision in the preceding sentence.

10.6 Upon termination of the Agreement for any reason whatsoever, (a) all sums due to SCM but not yet paid shall become immediately due and payable, (b) all rights and licenses granted to You under the Agreement will terminate, and (c) You shall destroy or return to SCM all copies of the Software, source codes and Documentation in Your possession and shall confirm this in writing towards SCM upon its first request. After termination of the Agreement, SCM is not obliged to furnish and/or to convert any information, material, or data to You.

10.7 If You did not make use of a free evaluation period before ordering Software, then You may cancel the Agreement free of charge if You find the Software unsatisfactory for whatever reason by giving written notice to SCM within 30 days after You have obtained download information from SCM. Article 10.6 is applicable to such cancellation.

10.8 All provisions relating to confidentiality and ownership shall survive the termination of these License Terms.

ARTICLE 11 CONFIDENTIALITY

11.1 The term “Confidential Information” means any information, in whatever form, disclosed by SCM that relates to the Software, including but not limited to the source code, the Data files and the Documentation, and that is not publicly known as well as any information, in whatever form, disclosed by SCM to You in connection with these License Terms that is identified as “confidential” or “proprietary” by SCM, or which You have reason to believe is treated as confidential or proprietary by SCM.

11.2 You agree to maintain and preserve the confidentiality of all Confidential Information in strict confidence, including, but without limitation, taking at least the same measures to protect and preserve the confidentiality of the Confidential Information as it takes to preserve and protect the confidentiality of Your own confidential information, but in any event taking no less than a reasonable degree of care. Furthermore You agree to disclose such Confidential Information to Your own employees and consultants on a “need-to-know” basis only, and only to those employees and consultants who have agreed to maintain the confidentiality thereof under terms at least as restrictive as those contained herein. Notwithstanding the foregoing and subject to article 5.2, You are entitled to publish the results obtained with the Software in scientific literature.

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14.1 As far as applicable law allows, in the event SCM is liable for any loss or damage suffered by You, as a result of an attributable breach by SCM or unlawful act or otherwise, expressly including a breach of a warranty, SCM will only be liable for the direct damages, strictly meaning (i) the reasonable costs made to have the SCM's performance meet with its obligations under the Agreement; and (ii) the reasonable costs to be made in order to prevent or to limit the damages caused; and (iii) the reasonable costs to determine the liability and the nature and scope of the damages; and (iv) the reasonable costs to be made in order to seek for any remedy out of court. The total damages shall not, however, in any case exceed the amount paid by You for the Software in the current calendar year and the two previous calendar years.

14.2 In no event shall SCM be liable for any indirect, special, incidental or consequential damages, whether under the Agreement or otherwise, including but not limited to loss of profits, loss of use, loss of or damage to data, or interruption of business, irrespective whether SCM has advance notice of the possibility of such damages.

14.3 No clause in these License Terms is intended to exclude the liability of SCM in case of gross negligence or wilful misconduct.

ARTICLE 15 THIRD PARTY SOFTWARE

15.1 You acknowledge and agree that the Software contains Third Party Software. Any such Third Party Software falls under the scope of these License Terms.

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You agree that the Software is not being and will not be acquired for, shipped, transferred, or re-exported, directly or indirectly, to proscribed or embargoed countries or their nationals, nor will it be used for: nuclear activities, chemical or biological weapons, or missile projects unless authorized by the Dutch government. You warrant that You are not located, nor under the influence of, a country embargoed by The Netherlands or the US.

ARTICLE 17 MISCELLANEOUS

17.1 If any term or provision of these License Terms shall be found to be illegal or unenforceable, then, notwithstanding that term, all other terms of these License Terms will remain in full force and effect and parties shall substitute the affected term or provision for an enforceable term or provision which approximates the intent and economic effect of the affected provision.

17.2 The failure by SCM to exercise any right hereunder shall not operate as a waiver of SCM's rights to exercise such right or any other right in the future.

17.3 The Agreement and the use of the Software will be governed by the laws of The Netherlands.

17.4 To the extent that national or international rules of law do not prescribe mandatory conditions to the contrary, any and all disputes arising from or related to the Agreement and these License Terms will be brought before the competent court in Amsterdam.

17.5 The Vienna Sales Convention of 1980 shall not apply.

17.6 These License Terms replace any earlier License Terms or End User License Agreement (EULA) You may have signed with SCM. Any older License Terms or EULA hereby become null and void.

License Terms, version 5 September 2014 with minor change in article 1 (new trade name of SCM)