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The VASP Software GmbH (“VG” in the following) and the

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(“Licensee” in the following) conclude the following Agreement:

1. Grant of license, scope of license

1.1. Subject to the terms and conditions of this Agreement, the Licensee acquires a non-exclusive perpetual academic or non-profit license for the use of the software-package VASP (Vienna ab-initio simulation package) for ab-initio total-energy and molecular-dynamics calculations, version VASP 5.4.4 an VASP.6.4 for the research group:

.....²

1.2. Under this license the use of the software is restricted to a maximum of 6 (six) named users (researchers or students), all belonging to this research group and to the same organizational unit and working at the same location. The license does not cover the use of VASP by collaborators working in other research groups, organizational units or institutions.

1.3. The license covers access to the VASP software. The VASP software includes the source-code, the program documentation, and the data-base for pseudopotentials and PAW-potentials (in the following PP-data-base), as well as any VASP executables obtained by download or by compiling the source code. VG shall retain all right, title, copyright and other proprietary and intellectual property rights in the VASP software. Licensee does not acquire any rights other than those specified in this Agreement.

2. Transfer prohibited, no access to third parties

2.1. The license is not transferable to any other research group of the licensee or a third party without the prior written consent of VG. VG reserves the right to refuse authorization of such a transfer.

2.2. Licensee may not rent out, lease, sell or sublicense the VASP software or any part thereof. The Licensee guarantees that the VASP software or parts thereof shall not be made accessible to third parties without the explicit written consent of VG.

2.3. All installations of the VASP software must be accessible only to the authorized named users. Installation of VASP software on the cloud is only allowed, if the cloud provider guarantees full protection of the VASP software against access by unauthorized users, and if the terms of the cloud provider do not infringe any of the rights set out in this Agreement.

3. Delivery of the source-code and PP-data-base

3.1. Access to the code and to the PP-data-base shall be made available through a download account of the VG after the licence fee has been paid in full to VG.

¹ Please insert here the name of the institution concluding this agreement with the VG. This institution must be a legal person and the agreement must be signed by an authorized representative.

² Please insert here the name and affiliation of the research group for which the license is acquired.

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- 3.2. The Licensee guarantees that the password for this account will be known only to one primary contact-person and shall not be communicated to anyone else. The Licensee will be liable for any losses incurred by VG caused by the violation of this clause.

4. Administration of users, electronic database

- 4.1. VG will store the names, addresses, and email addresses of the Licensee, research group leader, primary contact person and of the named users, who are authorized to use the VASP software, electronically in a database. For that purpose the names and email addresses of the users must be communicated by the research group to VG. The primary contact person can delete and add new users, as long as the licensed number of users is not exceeded.
- 4.2. Postings on the user forum or access to precompiled VASP executables on high performance computer centres are restricted to registered named users only. VG can use the database to communicate updates, bug fixes, and VASP related events to the research group leader and primary contact-person. Upon request, the name of the signatories and primary contact-person will be removed from the database. In this case it will no longer be possible to access the download account of VG and the Licensee will not receive access to any further updates and new releases of VASP.6.X. The Licensee can continue to use already downloaded copies of the software as long as the contract is not infringed.

5. Benchmarks

- 5.1. If the Licensee uses the VASP software for benchmarking, numbers must be kept confidential and the results of the benchmark tests must not be published or communicated to third parties without written permission of the VG.
- 5.2. After prior written permission of the VG, benchmarks may be also performed by external staff or companies, if the Licensee can ensure that access to the code is for a limited period and limited to persons involved in the benchmarking. The Licensee must also ensure that the external staff or company will remove all their copies of the VASP software after benchmarking.

6. Modifications, add-ons

If the VASP software is modified in any way, for instance if new routines are added or existing routines or algorithms are modified the Licensee agrees to make these modifications available to VG. VG receives a non-exclusive, perpetual license to use these software-developments, including the right to include them in future releases of VASP, modify, distribute and sublicense these modifications or transfer this non-exclusive license to any other entity. If VG does not intend to include the modifications in future versions of VASP, VG may give an explicit written consent to the Licensee to distribute the modifications as add-ons. Add-ons are modifications or additions to the functionality of VASP that are executed by the main code and use part of the VASP source code. The add-ons must be distributed under an appropriate license not infringing the rights laid out in this Agreement. Distribution of the add-ons under a copyleft license (e.g. GPL) is explicitly forbidden.

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7. Copyright notice

In future publications of work performed using VASP, the use of the software shall be properly acknowledged, e.g. in the form

"The calculations have been performed using the Vienna ab-initio simulation package VASP.X.x [1,2]."

[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11 169 (1996).

If the PAW potentials are used, reference shall be made to

[2] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).

If special features implemented in VASP have been used, relevant publications as listed in the VASP documentation shall be cited.

8. License fee, payment terms

- 8.1. The Licensee accepts to pay to VG a license fee of Euro 5000,- (fivethousand Euro) promptly after the signature of this Agreement. Any local taxes, sales taxes, value added taxes (if applicable), import fees, bank charges need to be covered by the Licensee and are not included in this fee.
- 8.2. This license fee is strongly discounted and applies only to academic institutions with undergraduate teaching or non-profit research institutions. The Licensee may use VASP exclusively for non-profit research. If Licensee wishes to use VASP in contractual research in cooperation with or for industry or military institutions, the conditions will have to be renegotiated.
- 8.3. In the event of default in payment, VG shall be entitled to charge default interest in the amount of 8% per annum. In addition, the Licensee must reimburse all dunning and collection expenses and legal fees incurred and necessary for the appropriate legal prosecution.

9. Termination

- 9.1. The license may be terminated by VG with immediate effect for good cause, if the Licensee fails to comply with any material provision of this Agreement, in particular, if the Licensee infringes VG's copyrights or if the license fee is not paid in full despite a reminder and expiration of a reasonable grace period.
- 9.2. In case of termination, the Licensee must delete all copies of the software that are in his possession or control and has no claim to reimbursement of payments made. All provisions of this Agreement relating to disclaimers of warranties, limitation of liability and all of VG's proprietary rights shall survive termination.

10. Maintenance, support

The license does not cover any maintenance service for the software or support, although, complimentary updates to new releases of VASP.6.X will be made available without additional charge for 3 years after the date of the signature of this Agreement.

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12. Liability

To the maximum extent permitted by applicable law, VG declines any liability for the software and any responsibility for the results of calculations produced by the VASP software package. VG shall generally be liable to the Licensee only for intentional and severe grossly negligent breach of its contractual obligations. VG’s liability shall be limited to typically predictable damage which the Licensee has incurred and, in terms of amount, shall be limited to the license fees actually paid by Licensee. VG shall not be liable in any event for lost profits, indirect or consequential damages including lost data and pure property damages of any kind.

13. Indemnification

Subject to the limitations provided for in clause 12 (liability), VG will defend and indemnify Licensee against a claim that the VASP software infringes upon any intellectual property right of a third party provided that: (a) Licensee notifies VG in writing within 14 days of the claim; (b) VG has sole control of the defence and all related settlement negotiations; and (c) Licensee provides VG with the assistance, information and authority necessary to perform VG’s obligations under this clause. VG shall have no liability for any claim of infringement based on the combination, operation or use of the VASP software licensed under this Agreement with other software, hardware or other materials not furnished by VG, if such infringement would have been avoided by the use of the VASP software without such software, hardware or other materials. In the event the VASP software is legally held or is believed by VG to infringe, VG shall have the option, at its expense and at its sole discretion, to alternatively: (a) modify the VASP software to be non-infringing or (b) obtain for Licensee a license to continue using the VASP software. Any further claims of Licensee shall be excluded.

14. Final Provisions

- 14.1. The terms of this Agreement shall prevail over any terms or conditions of the Licensee.
- 14.2. This Agreement shall be governed by and construed in accordance with Austrian law without reference to its conflict of law rules. The application of the United Nations Convention on Contracts for the International Sale of Goods is hereby expressly excluded.
- 14.3. Any disputes arising from or in connection with this Agreement shall exclusively be referred to the competent court in Vienna which has subject-matter jurisdiction.
- 14.4. If any provision of this Agreement shall be declared invalid, void, or unenforceable, the validity and binding effect of any remaining portion will not be affected, and the remaining portions of this Agreement will remain in full force and effect as if this Agreement had been executed with

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said provision eliminated. The invalid provision shall be replaced by a provision which comes as close as possible to the will of the parties within the framework of what is legally possible and which best corresponds in its economic effect to the invalid provision.

For the VASP Software GmbH:

Georg Kresse
Berggasse 21/14, A-1090 Wien, Austria

Signature and Date:

For the Licensee

Name and capacity in which acting:

Institution:

Address of Institution:

Signature and Date:

The research group leader and the primary-contact-person responsible for the installation of VASP herewith confirm that they have read the contract in full. They understand that under this license access to VASP is restricted to 6 named users and that the password to the VG download account must not be shared with anyone for whatsoever reason.

For the research group entitled to use VASP

Research group:

Address of Research group:

Name:

Signature and Date:

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Primary-contact-person responsible for the installation of VASP at the institution
(leave blank, if the primary contact-person and the signatory for the research group are identical)

Name:

Signature and Date:

