

## SOFTWARE LICENSE AGREEMENT FOR THE USE OF VASP5.2 BY ACADEMIC INSTITUTIONS

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The Universität Wien, Austria (UW in the following) and the  
Wake Forest University, Winston-Salem, NC, USA  
(WFU in the following) <sup>1</sup> conclude the following agreement:

(1) The WFU acquires a non-exclusive academic license for the use of the software-package VASP (Vienna ab-initio simulationprogram) for ab-initio local-density-functional total-energy and molecular-dynamics calculations, versions VASP5.2 and VASP4.6, by the research group Condensed Matter Group of WFU Physics Department <sup>2</sup> Under this licence the use of the software is restricted to a maximum of six researchers or students, all belonging to this research group and to the same organisational unit and working at the same location. The licence does not cover the use of VASP by external collaborators working at other institutions.

(2) The license covers access to the source-code, the program documentation and to the data-base for ultrasoft pseudopotentials and PAW-potentials. UW reserves the exclusive property of the software. It declines any liability for the software and any responsibility for the results of calculations produced with the program. The license does not cover any maintenance service for the software or support for its implementation.

(3) The license is not transferable to another research group of WFU without the written agreement of UW. UW reserves the right to refuse authorization of such a transfer. A transfer to a research group not belonging to WFU is excluded.

(4) The WFU guarantees that the software or parts thereof shall not be made accessible to third parties without the explicit written consent of UW. Access to the code and to the data-base shall be made available through an account of the UW. The WFU guarantees that the password for this account and any of its modifications will be known only to one contact-person and shall not be communicated to temporary co-workers or guests. All installations of the source code, the executable or the data-base must be copy-protected and accessible only to the authorized users.

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<sup>1</sup>Please insert here the name of the institution concluding this agreement with UW. This institution must be a legal person and the agreement must be signed by an authorized representative of this institution. Define the acronym (replacing ..... ) under which this institution is referred to in the text of the agreement.

<sup>2</sup>Please insert here the name and affiliation research group for which the license is acquired

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(5) If the Licensee uses the VASP code 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 University of Vienna. After prior written permission of the University of Vienna, benchmarks may be performed by external staff 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 will remove all copies of the code after benchmarking.

(6) If VASP is used as the basis of further methodological or software-development, WFU agrees to make these additions available to UW. UW will also be entitled to include these additions in further releases of VASP.

(7) 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 ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) developed at the Institut für Materialphysik of the Universität Wien [1,2]."

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

If the PAW-version is used, reference will be made to

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

If special features implemented in VASP will have been used, reference should be made to the relevant publications as listed on the VASP home-page.

(8) The WFU accepts to pay to UW a licence fee Euro 4.000,- (fourthousand Euro). The licence fee is strongly discounted and applies only to academic institutions with undergraduate teaching.

(9) The licensee will use VASP exclusively for non-profit research. If VASP is used in contractual research in cooperation with or for industry or for military institutions, the financial conditions will have to be re-negotiated.

(10) UW declares that it has the full power and authority to grant the rights granted in this agreement without the consent of any other person, and that the license and use of the software by the licensee will not in any way constitute an infringement or other violation of any copyright, proprietary right or any other rights of any third party.

(11) Any disputes arising from the license agreement are subject to the laws and jurisdiction of the Republic of Austria.

(12) The terms of this agreement shall prevail any terms or conditions of the licensee.