



**The following is an excerpt of the full FHI-aims license agreement that was agreed on and executed between MS1P and the original licensee (academic group leader who licensed FHI-aims). The following terms apply to each user in the groups that licensed FHI-aims, and each user must adhere to these terms in order to download / use any FHI-aims related material made available to them.**

Excerpt from the agreement by and between

Molecular Simulations from First Principles (MS1P) e.V.  
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– as licensor, hereinafter referred to as "MS1P" –

and

– as licensee, hereinafter referred to as "YOU" –

– MS1P and YOU hereinafter individually also called a "Party", and collectively also called the "Parties" –

## **Preamble**

A. MS1P is coordinating the development of the software "FHI-aims" (Fritz Haber Institute *ab initio* molecular simulations, hereinafter the "Software") and licenses the Software. The Software is a computer program package to calculate physical and chemical properties of condensed matter, based on a first-principles quantum-mechanical description of the electronic structure, as specified below.

The primary production method is density-functional theory. The Software is also a flexible framework for advanced approaches to calculate ground- and excited-state properties. Current developments include hybrid functionals, Hartree-Fock and Møller-Plesset perturbation theory (MP2), QM/MM, and many-body perturbation theory (*GW* selfenergies).

The Software uses numeric atom-centered orbitals as the quantum-mechanical basis set. This enables accurate all-electron, full-potential calculations at a computational cost which is competitive with, for instance, plane wave pseudopotential methods, without



invoking a priori approximations to the potential (such as e.g. pseudopotentials, frozen cores).

The initial development of the Software has been performed at the Fritz-Haber-Institut ("FHI"), an institute of the Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. ("MPG"), a German non-profit scientific research organization. MPG has transferred the right to use and exploit the Software to MS1P. In recent years a wider community has been and continues to contribute to the further development of the Software. MS1P has been granted the right to use and exploit such developments based on agreements similar to Section 1.4 below.

- B. MS1P has agreed with YOU to grant YOU a license to use and exploit the Software subject to the terms and conditions of this License Agreement ("Agreement"). The Software is to be used for the 71 solids and the PBE functional described in K. Lejaeghere, et al., Reproducibility in density functional theory calculations of solids. *Science* 351, aad3000 (2016) ("PURPOSE"). All other features, mentioned above and added in the future are "under development" and this is why the Software is provided as source code. Using any of them is at the sole risk of the YOU.
- C. Notwithstanding the details set forth below and in order to emphasize the importance of the following, YOU are aware that the Software has been developed with great care for academic purposes and has been carefully tested (K. Lejaeghere et al., cited above). Nonetheless, MS1P does not make any warranty for its functionality, neither express nor implied.

Now, therefore, the Parties agree as follows:

## **1. Grant of Rights**

- 1.1 MS1P herewith grants YOU a non-exclusive, non-transferable, non-sublicensable worldwide, fee-based license to use the Software for the PURPOSE subject to the terms of this Agreement.
- 1.2 Any use of the Software for purposes other than the PURPOSE, in particular any commercialization (e.g. sale, lease, license) of the Software, is not allowed. The use of the Software by or on behalf of third parties is not permitted.
- 1.3 YOU may copy the Software if required for security backup purposes. Copyright notices and marks shall not be deleted, modified, and/or eliminated. Copies that are no longer needed shall be deleted or destroyed. Back-up copies shall be deleted at the end of the term of this Agreement.
- 1.4 YOU are entitled to modify the Software. If the Software is modified by YOU, YOU herewith grant, where legally entitled to grant, MS1P a non-exclusive, worldwide,



perpetual, irrevocable, sub-licensable and royalty-free license to such modifications of/within Software. MS1P shall be entitled to use (including but not limited to save, load, run, display, exhibit, publish and copy) and to alter, translate, adapt or otherwise modify such modifications, and to distribute such modifications and improvements (in original or altered, translated, adapted or otherwise modified form) together with the Software and any future updates/upgrades of the Software. The ownership rights in and to such modifications shall remain with the developers of such modifications.

- 1.5 The Software for the PURPOSE is limited at any one time to the number of users as set forth in the original agreement. We ask that each user registers at the FHI-aims website <http://www.fhi-berlin.mpg.de/th/aims>. This also ensures that they receive information about bug-fixes, add-ons, and updates. Please note that licensing options are also available beyond five users, e.g., up to 20 users, or negotiable for larger needs.
- 1.6 YOU have to ensure that the users are aware of and comply with the terms of use contained in this Agreement. YOU have to ensure that unauthorized use is not possible.
- 1.7 The Software can include open source software components to the extent that this does not inhibit the contractual use of the Software. Open source software that MS1P provides to YOU is primarily subject to the corresponding open source license terms and conditions that are indicated in the system requirements of the Software.
- 1.8 Citation of the Computer Physics Communications publication on FHI-aims. In any publication relating to FHI-aims, YOU shall give proper scientific credit to FHI-aims, for example in the following form: "The calculations have been performed using the FHI-aims package [1]."  
[1] Volker Blum, Ralf Gehrke, Felix Hanke, Paula Havu, Ville Havu, Xinguo Ren, Karsten Reuter, Matthias Scheffler, Comp. Phys. Comm. 180, 2175-2196 (2009).

## **2. Services of MS1P**

### 2.1

2.2 YOU will be provided with a user manual in electronic format.

2.3 Any other services beyond the provision of the Software, such as consulting, installation, launch, parameterization, customizing, migration, training, programming work and other customer-specific project services will only be due if expressly agreed upon in a separate contract.

2.4 MS1P shall not have any obligation to support YOU during the term of this Agreement with respect to Software and any problems or defaults that may occur in connection therewith. Support services and other services not specified in this Agreement are only



due if the Parties have concluded a respective separate agreement, in particular regarding the additional remuneration.

### **3. No Warranties and Representations / Indemnification**

- 3.1 MS1P makes no representations or warranties of any kind concerning the Software, express or implied, and the absence of any legal or actual defects, whether discoverable or not. Specifically, and not to limit the foregoing, MS1P makes no warranty or representation regarding the merchantability or fitness for a particular purpose of the Software.
- 3.2 YOU shall indemnify, defend and hold harmless MS1P and its trustees, officers, employees, students, guests, and agents (collectively "Indemnitees"), against any liability, damage, loss, or expense (including reasonable attorney fees and expenses) incurred by or imposed upon any of the Indemnitees in connection with any third party claims, suits, actions (including without limitation actions in the form of tort, warranty or strict liability and regardless of whether such action has any factual basis), demands or judgments arising out of or in connection with any use of the Software by YOU, except in case of gross negligence or willful misconduct of MS1P.
- 3.3 To the extent legally permissible, MS1P, their respective trustees, directors, officers, students, employees and agents, and their respective successors, heirs and assigns, shall not be liable for incidental or consequential damages of any kind, including but not limited to economic damages or injury to property and lost profits, except in case of gross negligence and willful misconduct of MS1P.

### **4. Financial Provisions**

#### **5. Term and Termination**

- 5.1 This Agreement shall come into effect on the date of signature of this Agreement by the Party last to sign (the "Effective Date"), and shall be valid valid for a period as set forth in the actual agreement.
- 5.2 The right to terminate for cause remains unaffected. Any material breach of this Agreement by a Party shall entitle the other Party to terminate this Agreement if the defaulting Party fails to remedy such breach within thirty (30) calendar days after receipt of a written notice specifying the breach and requiring its remedy. For MS1P cause shall exist, in particular without limitation, if YOU are in default with the payment of the license fees for more than two months.
- 5.3
- 5.4 Any notice of termination shall be given in the written form pursuant to sec. 126 para 1 BGB (German Civil Code), i.e. a signed letter, to be effective.



5.5 The provisions set forth in Sections 1.4, 3, 5.5, 5.6, 6.4 and 6.6 shall survive the termination of the Agreement.

5.6 After the termination of the Agreement, YOU shall cease any use of the Software and, upon request of MS1P, shall destroy all copies of the Software or return to MS1P all copies of the Software. MS1P may request a written declaration that YOU have complied with the request.

## **6. Miscellaneous**

6.1 This Agreement shall exclusively govern the licensing of the Software by YOU. Other terms and conditions shall not apply, even if MS1P does not expressly object to them. In particular, but not limited to, this shall apply to terms and conditions for purchase by YOU.

6.2 This Agreement shall inure to the benefit of the Parties and shall be binding upon their legal successors.

6.3 This Agreement is personal to YOU and no rights or obligations may be assigned by YOU to a third party without the prior written approval of MS1P, which consent shall not unreasonably be withheld.

6.4 This Agreement shall be construed, governed, interpreted and applied in accordance with the laws of the Federal Republic of Germany (without its conflict of laws rules).

6.5 No modifications or supplementations of this Agreement shall be effective unless in writing and signed by both Parties. Should one of the provisions of this Agreement be void, invalid or unenforceable, the remaining provisions of this Agreement will not cease to be effective. The Parties shall negotiate in good faith to replace such void, invalid or unenforceable provision by a new provision that reflects, to the extent possible, the original intent of the Parties.

6.6 The Parties shall attempt to settle any dispute or claim arising out of or relating to this Agreement by good faith negotiations within a reasonable period. If the Parties are unable to settle, claims or controversies under this Agreement, the enforcement or interpretation hereof, or any alleged breach or default under the provisions hereof, such claims or controversies shall exclusively be settled by the court competent for the registered office of MS1P.