

The following is an excerpt of the full FHI-aims license agreement that was signed and executed between MI 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.

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**License Agreement**  
(hereinafter the “**Agreement**”)

by and between

Max-Planck-Innovation GmbH  
Marshallstraße 8  
80539 München  
Germany  
Fax: +49-89-290 919 99

- as licensor, hereinafter referred to as “**MI**” -

and

- licensee, hereinafter referred to as “**YOU**” -

- MI and YOU hereinafter individually also called a “**Party**”, and collectively also called the “**Parties**” -

## Preamble

**A.** “FHI-aims” (Fritz Haber Institute ab initio molecular simulations) 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.

The primary production method is density functional theory. FHI-aims 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).

FHI-aims 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 methods, without invoking a priori approximations to the potential (such as pseudopotentials, frozen cores).

**B.** FHI-aims has been developed at the Fritz-Haber-Institut in Berlin (“**FHI**”), an institute of the Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. (“**MPG**”), a German non-profit scientific research organization. By agreeing to the following license, YOU obtain a personal license to use FHI-aims for non-commercial scientific research purposes, covering a small research group (up to five people). Notwithstanding the details set forth below, MI would like to emphasize the following important conditions of this license:

**No redistribution.** YOU are not allowed to redistribute FHI-aims in any way. FHI-aims represents a significant and continuing investment in time and effort on the part of its developers at FHI. Please refer any Third Parties interested in using FHI-aims to MI and the FHI-aims web site <http://www.fhi-berlin.mpg.de/th/aims>

**No warranty.** FHI-aims has been developed by FHI with great care, and is a capable tool for FHI's own research purposes as well as those of others. Nonetheless, as set forth below, neither MI, nor MPG, nor FHI can make any warranties for its functionality, either express or implied.

**Grant-back license.** If YOU make modifications or improvements to FHI-aims, MI asks YOU to make any such modifications or improvements available to MI and FHI as set forth below, so as to allow MI and FHI to use and redistribute them with FHI-aims in the future. It is the aim of FHI to keep a single version of FHI-aims accessible to all users, and this provision shall ensure that this can be done. Please be ensured that your contribution will be referenced appropriately.

**Please cite the Computer Physics Communications publication on FHI-aims.** In any published research with FHI-aims, please give proper scientific credit to FHI-aims 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, Computer Physics Communications [volume], [page] (2009).

Now, therefore, the Parties agree as follows:

## **Article 1 - Grant of Rights**

### 1.1 License Grant

MI herewith grants to YOU a non-exclusive, worldwide, royalty-bearing license to use FHI-aims for non-commercial, scientific research purposes. YOU are not allowed to grant sublicenses under FHI-aims to any Third Parties. “Third Parties” shall mean any person or entity other than MI and YOU.

This license grant includes the following rights of use:

a) Installation of FHI-aims and use of the installed FHI-aims by maximally five (5) users working in your academic group.

All users must register at the FHI-aims web site <http://www.fhi-berlin.mpg.de/th/aims>. This also ensures that they receive information about bug-fixes, add-ons, and updates. And it legitimates them to join the FHI-aims users club. Reasonable care has to be taken by YOU that unauthorized use is not possible. In case of installation of FHI-aims on multi-user hardware or on a network, YOU have to ensure that only authorized users can use FHI-aims.

b) Access to the copyrighted FHI-aims user manual which is made available to registered users under <http://www.fhi-berlin.mpg.de/th/aims>

c) Modification of FHI-aims in order to adapt FHI-aims to your IT-infrastructure. YOU are allowed to use the results of such modifications in accordance with section a) above.

d) Realization of new functionalities of FHI-aims in accordance with section 1.4 below.

### 1.2 Limitations of License Grant

YOU are not allowed

a) to copy FHI-aims (neither in whole nor in part, neither permanently nor temporarily, neither in its original version nor in any modified version), if and to the extent such copying is not necessary for the agreed use of FHI-aims according to section 1.1 of this Agreement;

b) to distribute (neither commercially nor free of charge, neither permanently nor temporarily) FHI-aims (neither in whole nor in part, neither in its original version nor in any modified version) or any copies thereof to Third Parties;

c) to grant Third Parties the right to use, modify, copy and/or distribute FHI-aims (neither in whole nor in part, neither permanently nor temporarily, neither in its original version nor in any modified version) or any copies thereof; and

d) to include FHI-aims (neither in whole nor in part, neither permanently nor temporarily, neither in its original version nor in any modified version) or any copies thereof into any other programs without the prior written approval of MI and FHI.

### 1.3 Transfer of FHI-aims and Source Code / No Support by MI, MPG or FHI

Access to the code shall be made available through an ftp-account of FHI. YOU shall guarantee that the password for this account will be treated confidentially, and shall not be communicated to any temporary co-workers or guests.

Neither MPG, nor FHI, nor MI shall have any obligation to support YOU during the term of this Agreement with respect to FHI-aims and any problems or defaults that may occur in connection therewith.

#### 1.4 Grant-back

If FHI-aims is used as the basis for further scientific developments, YOU shall grant FHI and MI a non-exclusive, world-wide, irrevocable, royalty-free license to any resulting modifications and improvements of/within FHI-aims. FHI and MI shall be entitled to use such modifications and improvements, and to distribute such modifications and improvements together with FHI-aims and any future updates/upgrades of FHI-aims. The ownership rights in and to such modifications and improvements shall remain with the developers of such modifications and improvements.

### **Article 2 - No Warranties and Representations / Indemnification**

2.1 YOU are aware of the fact that FHI-aims (i) results from basic research, (ii) has not undergone complete testing and (iii) may contain errors.

2.2 MI, FHI AND MPG MAKE NO REPRESENTATIONS OR WARRANTIES OF ANY KIND CONCERNING FHI-AIMS, EXPRESS OR IMPLIED, AND THE ABSENCE OF ANY LEGAL OR ACTUAL DEFECTS, WHETHER DISCOVERABLE OR NOT. Specifically, and not to limit the foregoing, MI, FHI and MPG make no warranty or representation (i) regarding the merchantability or fitness for a particular purpose of FHI-aims and (ii) that the use of FHI-aims will not infringe any patents, copyrights or other intellectual property rights of a Third Party, and (iii) that the use of FHI-aims will not cause any damage of any kind to YOU or a Third Party.

2.3 YOU shall indemnify, defend, and hold harmless MI, FHI and MPG and their trustees, officers, directors, students, employees and agents, and their respective successors, heirs and assigns (the "Indemnitees"), against any liability, damage, loss, or expense (including reasonable attorneys fees and expenses) incurred by or imposed upon any of the Indemnitees in connection with any claims, suits, actions, demands or judgments arising out of any liability (including without limitation actions in the form of tort, warranty, or strict liability and regardless of whether such action has any factual basis) in connection with any use of FHI-aims.

### **Article 4 – Further Obligations**

4.1 YOU shall ensure that the source code of FHI-aims and the FHI-aims user manual provided by FHI to YOU under this Agreement will be stored in a secure environment, and that no Third Party (including but not limited to unauthorized personnel of YOU) has access to the source code or executables.

4.2 Publications of work performed using FHI-aims shall properly acknowledge the use of FHI-aims, e.g. 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, Computer Physics Communications [volume], [page] (2009)

### **Article 5 - Term and Termination**

5.1 This Agreement shall be valid for a period of ten (10) years. After this term, the Parties shall discuss in good faith whether to extend this Agreement or not.

5.2 Any material breach of this Agreement by a Party shall entitle the other Party to terminate this Agreement after one (1) month prior written notice 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.

- 5.3 If YOU are adjudicated bankrupt or become insolvent, this Agreement shall terminate automatically.
- 5.4 The provisions set forth in Article 1.4, 2, 4.2, 5.4, 5.5, 6.3 and 6.5 shall survive the termination of the Agreement.
- 5.5 After the termination of the Agreement, YOU shall cease any use of FHI-aims and, upon request of MI, shall destroy or return to MI FHI-aims and the source code.

#### **Article 6 - Miscellaneous**

- 6.1 This Agreement shall inure to the benefit of the Parties and shall be binding upon their legal successors.
- 6.2 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 MI, which consent shall not unreasonably be withheld.
- 6.3 This Agreement shall be construed, governed, interpreted and applied in accordance with the laws of the Federal Republic of Germany.
- 6.4 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 held 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.
- 6.5 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 MI.