

# AGREEMENT FOR THE USE OF HT-CADSS SOFTWARE PACKAGE

**HT-CADSS** stands for High-Throughput-based Complex Adsorption and Diffusion Simulation Suite), which was developed under the collaboration of Prof. Qingyuan Yang and Chongli Zhong at Beijing University of Chemical Technology. This software package was written in a serial manner using Fortran 90 language, and all the subroutines and functions were encapsulated into modules from which the code can be easily extended if necessary. The current version of HT-CADSS (V2.2) can perform Monte Carlo and Molecular Dynamics simulations in various ensembles. It is applicable to simulate the adsorption and diffusion behaviors of pure fluids and mixtures in various nanoporous crystalline materials as well as materials structure characterization.

To better promote the development of computational materials science, we decided to open this software package for scientific researchers with a free usage, under the specific terms in this agreement. On the basis of an abidance by these terms, the applicants can fill the information required in the following Table and send it back to us. Then, we will give you the detailed information to get a copy of this software package. Once you download, copy, visit, or install HT-CADSS, it means that this agreement starts to take effect between you and our group.

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## 1. Applicant Information

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## 2. Specific Terms of This Agreement

- 1) This software package (including but not only limited to the contained images, added-on programs, explanatory materials such as user manual), and any updates for the original copy sent to the users, are owned by our group.
- 2) This software can only be used for the purposes of scientific research, MUST not for commercial behaviors.

- 3) Without our permission, HT-CADSS can be transferred to any other persons beyond the authorized users.
- 4) Because HT-CADSS is provided free of charge, the entire risk as to the quality and performance of the software package is with you. Thus, we assume no responsibility for all the consequences brought by the use of this software.
- 5) We do not undertake any responsibility and obligation for guiding how to use the provided software packages.
- 6) If the authorized users publish any results obtained from HT-CADSS in any Journals or other medium, the use of this software package must be clearly declared in the main text of the published papers or materials, together with a citation of the following two information:
  - a) Qingyuan Yang and Chongli Zhong. High-Throughput-based Complex Adsorption and Diffusion Simulation Suite (HT-CADSS), Beijing University of Chemical Technology; Copyright No.: 2016SR110434, China.
  - b) Qingyuan Yang, Dahuan Liu, Chongli Zhong and Jian-Rong Li. Development of Computational Methodologies for Metal–Organic Frameworks and Their Application in Gas Separations. Chem. Rev. 2013, 113, 8261–8323.