## **MCNOX User License Agreement**

(ver. May, 2023)

MCNOX is a package developed by <a href="Prof. Weijie Hua">Prof. Weijie Hua</a> (wjhua@njust.edu.cn, Nanjing University of Science and Technology, China), <a href="Prof. Yi Luo">Prof. Yi Luo</a> (yiluo@ustc.edu.cn, University of Science and Technology of China, China), and <a href="Prof. Shaul Mukamel">Prof. Shaul Mukamel</a> (smukamel@uci.edu, University of California, Irvine, USA), which is capable of computing ultrafast (attosecond and femtosecond) nonlinear X-ray spectra of molecules at the multiconfigurational quantum chemistry level and analyzing the major transitions in terms of the natural transition orbitals. A manual is still under development. An introduction paper to the package is currently under review. More information and updates can be found via <a href="https://iszy.njust.edu.cn/lxy/hwj\_en/list.psp">https://iszy.njust.edu.cn/lxy/hwj\_en/list.psp</a> (Click the button "Research Project").

To use MCNOX, please complete this form, sign, and email the PDF to wihua@njust.edu.cn (W.H.).

For students, please ask the principal investigator (PI) to sign the form, and the code can be used for any members of the research group.

## I hereby confirm that:

- 1. I will NOT redistribute the package to a third party.
- 2. I will NOT use the package for any commercial use.
- 3. I will cite the package as follows:

Hua, W.; Luo, Y.; Mukamel, S. *Multi-Configurational methods for ultrafast NOlinear X-ray spectra (MCNOX)*, version 1.0; 2019.

4. I understand that there could be bugs in the code, and I will be responsible for the result.

Title	First Name (Middle Name)	Surname	Signature
Institute			
Department			Date (YYYY/MM/DD):
Address			
Country		Email	