



The Sir Martin Wood Prize Lecture



Development of Open Source Software for Phonon Properties in Materials Science

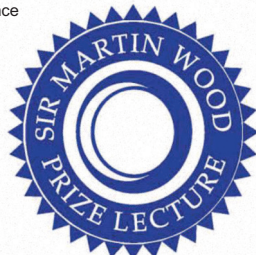


Atsushi Togo
National Institute for Materials Science, Japan

Biography

1994 – 1998 Kyoto University (B. Eng)
1998 – 2001 Kyoto University (M. Eng)
2003 – 2006 Dept of Materials Science and Engineering, Kyoto University (Ph. D)

Oct. 2006 – Mar. 2007
Postdoctoral Research Associate at Department of Materials Science and Engineering, Kyoto University
Apr. 2007 – Mar. 2008
Postdoctoral Research Associate at Institut für Anorganische Chemie, RWTH Aachen, Germany
Apr. 2008 – Jun. 2009
Postdoctoral Research Associate at Department of Materials Science and Engineering, Kyoto University
Jul. 2009 – Jun. 2010
Postdoctoral Research Associate at LEM ONERA-CNRS Châtillon in France
Jul. 2010 – Jun. 2012
Postdoctoral Research Associate at Department of Materials Science and Engineering, Kyoto University
Aug. 2012 – Jan. 2020
Program Specific Associate Professor at Elements Strategy Initiative for Structural Materials, Kyoto University
Feb. 2020 – Dec. 2022
Principal Researcher, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science
Jan. 2023 – present
Group leader, Center for Basic Research on Materials, National Institute for Materials Science



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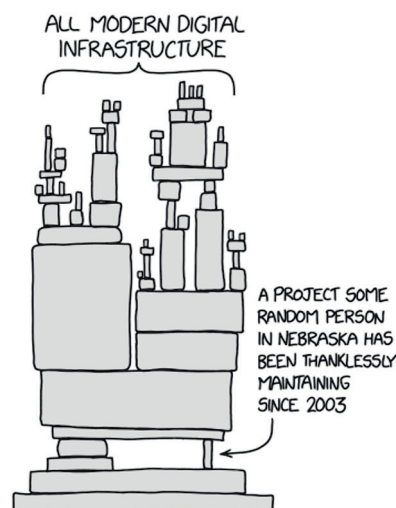
Friday, 8th September 2023
3:00 pm, Lecture Hall 2D5

MPI for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart (Germany)

Login data will be announced by email.

Growth of the semiconductor industry increases computer power exponentially. Our daily life is supported by accurate computer simulations as represented by weather forecasts. Computer simulations are realized by running software on computers. Many years ago, I started software development of a phonon calculation code, *phonopy* [1,2], for our own scientific interest.

By distributing it as open source software, many people started to use it. I also contribute to the software development of a crystallographic symmetry finder, *spglib* [3]. Since crystal symmetry is ubiquitous in solid state science, many other software projects rely on it like a comic shown below. Popular scientific software is infrastructure. I would like to present how we manage these scientific software projects in the modern era of the scientific community. Presently, I am interested in electron-phonon interaction calculation [4,5] and magnetic symmetry [6]. I would like to talk about our recent research activities.



- [1] A. Togo et al., J. Phys.: Condens. Matter **35**, 353001 (2023)
- [2] A. Togo, J. Phys. Soc. Jpn. **92**, 012001 (2023)
- [3] A. Togo and I. Tanaka, <https://arxiv.org/abs/1808.01590>
- [4] L. Chaput et al., Phys. Rev. B **100**, 174304 (2019)
- [5] M. Engel, et al., Phys. Rev. B **106**, 094316 (2022)
- [6] K. Shinohara, et al., <https://arxiv.org/abs/2211.15008>

Dr. Togo was awarded the Sir Martin Wood Prize at the Millennium Science Forum which took place in November 2021. The Millennium Science Forum was established in 1998 to promote scientific exchange between Britain and Japan and recognize the work of outstanding young Japanese researchers. The prize is named after Sir Martin Wood, founder of Oxford Instruments.