

§13. Study of Methods of Scientific and Industrial Application of Atomic and Molecular Data

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Recent fast, significant and remarkable advancement we have witnessed in past decades in areas such as high-tech. industries, medical research, environmental science, atmospheric science, fusion sciences as well as other basic sciences including astrophysics and radiation physics and chemistry fully depend on extensive utilization of atomic and molecular (A&M) data for structures basic understanding of various phenomena, but also establishing guiding new key principles and basic technologies based on simulations with this accurate and complete A&M data basis. Without this A&M data basis, such an impressive progress of our technologies and basic understanding of nature would not have been realized.

We undertook this collaborative effort to establish the forum as a platform connecting between A&M data producers and data users to integrate independent and isolated effort of data production and storage so that more efficient and complete data production and transmission could be possible.

In the present research project, we established a non-profit organization (NPO), named “The Forum for the Atomic and Molecular Data And Their Applications”. The certification of the forum was obtained on 13-Apr-2010 from the Gifu Prefectural government. The objectives of the forum is determined to be (1) the establishment of a community of producers of atomic and molecular data and users, (2) promotion of use of data in various fields from basic science to industrial applications, (3) establishment of a system to support operation of the data base.

For this purpose, we held meetings on May 13, June 7, June 22, October 3, 2011 and February 2 2012. Furthermore, we held a joint seminar on December 13 and 14, 2011, with the collaboration for meetings of NIFS titled, “Application of AM (atomic and molecular) data and AM model”, organized by Dr. H. Tanuma, on studies of plasma atomic

and molecular processes concerning to oxygen molecules. In the seminar, discussion was carried out to establish methods to estimate atomic and molecular data, which have not been obtained neither theoretically nor experimentally yet. It is realized that a large set of collisional radiative model has been constructed including estimated atomic and molecular data and multidimensional simulation of discharge has already been carried out. Discussion on this topic will be continued by organizing a working group.

We also discussed methods to promote communication between users and makers of atomic and molecular data using the internet. We have a web site and a mailing list based on google groups (<https://groups.google.com/forum/?hl=ja&fromgroups#!forum/pre-data-forum>), as shown in fig.1. Usefulness of the social networking services (SNS) is suggested. Methods for data maker to know data needs such as using a wish list are shown to be necessary, which can be realized if the members are joined the Facebook.



(fig.1) Web page of the google group for the forum for the atomic and molecular data and their applications (FAMDATA).

This year, a significant progress has been made for the modeling of high-Z multiple charged ions, which is useful for the studies of effects of high-Z impurities in the future fusion devices as well as light source applications. An international code comparison workshop (<http://nlte.nist.gov/NLTE7/>) was held and it was shown that the accuracy of the atomic data and completeness of the atomic model are essential for the modeling. Furthermore, comparisons between different codes are shown to be useful for the improvement of model, in such a situation that only limited experimental data is available. It is shown that the calculated mean charge and radiative power loss of tungsten agree well with experiments. The knowledge obtained by participating in this workshop will be applicable to the development of the general atomic and molecular databases.