The Franzosini Award of 2016

The 2016 Franzosini Award was given to David Fellhauer, in recognition of his contribution to the IUPAC Solubility Data Project, at the 15th Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data. Held in Geneva, Switzerland on 24 July 2016, the meeting occurred during the 17th International Symposium on Solubility Phenomena and Related Equilibrium Processes.

The recipient of the 2016 Franzosini Award David Fellhauer from KIT-INE with Clara Magalhães, Chair of the Subcommittee on Solubility and Equilibrium Data (SSED), during the conference dinner of the 17th ISSP, held in Geneva, Switzerland.

David Fellhauer is a young investigator working in the radiochemistry division of the Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal (KIT-INE), Karlsruhe, Germany. He is given this recognition in view of his outstanding scientific contribution to solubility behavior, aqueous speciation, and solid phase formation of actinide elements (especially Np and Pu) in different oxidation states. Based on his work, new comprehensive chemical and thermodynamic models have been derived for dilute to concentrated electrolyte solutions and various pH conditions. The studies provide a significantly improved scientific understanding of actinide solution chemistry and are of high relevance for assessing the long-term safety of nuclear waste repositories.

A Global Approach to the Gender Gap in Mathematical and Natural Sciences: How to Measure It, How to Reduce It?

One of three grants recently awarded by ICSU is to a new joint project led by the International Mathematical Union (IMU) and IUPAC, with the strong involvement of IUPAP. The project will compile evidence worldwide, including on trends on the role of

Who's Who in This New ICSU Project?

Lead Applicant 1

International Mathematical Union (IMU); Committee for Women in Mathematics Chair, Prof. Marie-Françoise Roy

Lead Applicant 2

International Union of Pure and Applied Chemistry (IUPAC); Bureau Member and past chair of the IUPAC Committee on Chemistry Education, Prof. Mei-Hung Chiu

Supporting Applicants

International Union of Pure and Applied Physics (IUPAP); Working Group 5 Chair, Prof. Irvy (Igle) Gledhill

International Astronomical Union (IAU); Women in Astronomy" Chair, Full Astronomer Francesca Primas

International Union of Biological Sciences (IUBS); Executive Director, Dr. Nathalie Fomproix

International Council for Industrial and Applied Mathematics (ICIAM); Past-President of ICIAM and Officer, Prof. Barbara Keyfitz

United Nations Educational, Scientific and Cultural Organization (UNESCO); Chief of the Section on Science Policy and Partnerships and member of the SAGA Steering Committee, Dr. Ernesto Fernández-Polcuch

Gender in Science, Innovation, Technology and Engineering (GenderInSite); Director, Prof. Alice Abreu

Support

ICSU Regional Offices in Africa and Latin America and the Caribbean

Observer

International Union of Theoretical and Applied Mechanics (IUTAM)

women in science, to support informed decisions and provide easy access to materials proven to be useful in encouraging girls and young women to study and work in scientific fields. With the involvement of six scientific unions, UNESCO, and GenderInSite, this project constitutes a large international and multidisciplinary collaboration.

Mathematical and natural sciences have long and honorable traditions of participation by highly creative women contributors. However, the percentages of scientists who are women remain shockingly low and there is a significant gender gap at all levels between women and men. Barriers to achievement by women persist, especially in developing countries. This project will produce sound data to support the choices of interventions that ICSU and member unions can feasibly undertake. Evidence will include trends, since the situation for women continues to change around the world, with some negative developments. Regional information about careers, jobs and salaries will also be provided. The Joint global survey is planned to reach respondents in more than 130 countries, using at least 10 languages, while the Joint study on publication patterns will analyze comprehensive metadata sources corresponding to the publications of more than 500,000 scientists since 1970. Contrasts and common ground across regions and cultures, less developed and highly developed countries, men and women, mathematical and natural sciences, will be highlighted.

The new ICSU grants, each worth 300,000 Euros across 3 years, created three international initiatives led by ICSU Unions. Through this program, ICSU's intent is to foster membership engagement by addressing long-standing priorities for ICSU Members in developing **science education, outreach and public engagement activities**, and by mobilizing resources for international scientific collaboration. In addition to the IMU/IUPAC grant described above, the following projects were awarded this year:

IUPAP-IUCr: Utilisation of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Conditions in Targeted Regions of the World

IUBS-INQUA: Trans-disciplinary Research Oriented Pedagogy for Improving Climate Studies and Understanding (TROP-ICSU)

www.icsu.org/what-we-do/projects-activities/icsu-grants-programme/grants-2016-2019

New InChI Software Release

The latest version of the InChI software, v1.05, has been released and is now available from http://www.inchi-trust.org/downloads/

In this version, the following features were added:

- Support for chemical element numbers 113-118
- Experimental support of InChI/InChIKey for simple regular single-strand polymers
- Experimental support of large molecules containing up to 32767 atoms
- Ability to read necessary for large molecules input files in Molfile V3000 format
- Provisional support for extended features of Molfile V3000
- Updated InChI API Library, including a novel API procedure for direct conversion of Molfile input to InChI and a whole new set of API procedures for both low and high-level operations (InChI extensible interface, IXA)
- Revised source code to ensure multi-thread execution safety of the InChI Library; several minor bugfixes/changes were made, and several convenience options were added to the inchi-1 executable.

The release is the first update since 2011 and the extended functionality is based on the outputs of IUPAC working groups.

While InChI provides a unique descriptor of molecular structures, the **Reaction-InChI** (RInChI) extends this idea towards reactions. Prototype versions of the RInChI have been available since 2011 (Grethe, Goodman and Allen, *Journal of Cheminformatics* 2013, 5, 45. DOI: 10.1186/1758-2946-5-45). The first official release (RInChI-V1.00) is also now available for download. This release defines the format and generates hashed representations (RInChIKeys) suitable for database and web operations. The RInChI provides a concise description of the key data in chemical processes, and facilitates the manipulation and analysis of reaction data.

Interested in learning more about InChI?
Consider attending the 2017 InChI meeting, 16-18 August 2017, in Bethesda, MD, USA. See more at https://iupac.org/event/chemical-identifier/

http://www.inchi-trust.org/