NIMS Award 2019 Goes to

Prof. Gerbrand Ceder and Dr. Pierre Villars

Overview

National Institute for Materials Science (NIMS) (Kazuhito Hashimoto, President) has selected the following scientists as the winners of the NIMS Award 2019.

Prof. Gerbrand Ceder
（**Professor, UC Berkeley**）

Dr. Pierre Villars
（**Director and Owner,
Material Phases Data System**）

NIMS Award 2019 will be given to two scientists who have done groundbreaking works in the field of "data-driven materials research and data infrastructure". Professor Gerbrand Ceder pioneered data-driven materials research based on the first-principles calculations. Meanwhile, Dr. Pierre Villars developed Pauling File, the world's largest inorganic materials database. Both research results have made a profound influence on the society as the comprehensive studies that have pioneered new avenues utilizing data in materials research or the research that became its solid foundation. The award ceremony and the NIMS Academic symposium will take place at the Tokyo International Forum on October 30 as a part of the NIMS WEEK 2019.

[NIMS Award]

Since 2007, the NIMS Award has been given to researchers around the world in recognition of their outstanding achievements in materials science and technology. This year's recipients were selected by the selection committee comprised of the staff members at NIMS and scientists from other organizations based on the nominations from the top scientists in the area of "Characterization, Simulation and Informatics"

[NIMS WEEK]

NIMS WEEK is an annual event hosted by NIMS consisting of Academic Symposium, Showcase and Open Laboratory. The participants can encounter "cutting edge materials research" through a variety of activities, such as the NIMS Award symposium to honor the award recipients and the exhibitions of the latest materials research at the NIMS Showcase. The largest ever "NIMS Open Laboratory"—which is mainly targeted towards industrial engineers and academic researchers including graduate students and faculty members—will be held on the first day of the NIMS WEEK to publicize the NIMS' research activities and may provide opportunities for collaborations, employment of graduate students and administrative staff members.

[NIMS WEEK 2019 Schedule]
October 28, Mon: NIMS Open Laboratory (NIMS, Tsukuba)
October 30, Wed: NIMS Award and Academic Symposium (Tokyo International Forum, Hall B5)
October 31, Thu: NIMS Showcase (Tokyo International Forum, Hall B5)
November 1, Fri: STAM 20th Anniversary Symposium (The Univ of Tokyo, San-jo Kaikan)

Awardee 1: Prof. Gerbrand Ceder (Professor, UC Berkeley)
Awardee 2: Dr. Pierre Villars (Director and Owner, Material Phases Data System)

Awardee 1: Prof. Gerbrand Ceder (Professor, UC Berkeley)

[Research field] Data-driven materials research

[Research achievement title] Pioneering data-driven materials research based on the first-principles calculations

[Research summary] Prof. Ceder has opened a new era of computational materials science by realizing the idea of linking the first-principles calculation data with statistical thermodynamics. He has demonstrated the power of materials design based on a large amount of computational data and pioneered data-driven materials research. Prof. Ceder has achieved outstanding results in the design and development of various functional materials, including lithium ion battery cathode materials, solid electrolytes, and thermoelectric conversion materials.

[Impact on the academic and industrial sectors] Prof. Ceder's idea on materials design based on a large amount of first-principles calculation data had great impacts on academia and industry. His work has led to the development of present computer data infrastructures dedicated to materials design. Prof. Ceder created a recent trend in materials development using data science.

Awardee 2: Dr. Pierre Villars (Director and Owner, Material Phases Data System)

[Research field] Fundamental research supporting data-driven materials research

[Research achievement title] Development of Pauling File, inorganic materials database

[Research summary] Dr. Villars advocated the concept of a database that organically links crystal structures, phase diagrams and properties of inorganic materials, and developed "Pauling File", a high quality and comprehensive world's largest inorganic materials database, from more than 180,000 documents published in over 1,000 scientific journals after year 1900 with unique curation method. As of July 2019, about 335,000 crystal structures, 44,000 state diagrams, and 400,000 properties have been recorded, and updates are ongoing.

[Impact on the academic and industrial sectors] 8 database products such as AtomWork and AtomWork Adv. provided by NIMS and Crystal Structure Data in PDF-4 + by ICDD, as well as 8 handbooks such as Landolt-Börnstein Handbook of Inorganic Substances (Springer) and Inorganic Substances Bibliography (DeGruyter) have been published based on the constructed inorganic materials database and are widely used throughout the world. In recent years, "data-driven materials research" using this database has been activated, and it is recognized as an important data resource to support the area.

(Reference) NIMS Award winners of the past six years and their achievements

2013   **Prof. Hideo Hosono** (Professor at Tokyo Institute of Technology, Japan)
"Discovery of iron-based superconductors and invention of IGZO-TFT"

2014   **Prof. Krzysztof Matyjaszewski** (Professor at Carnegie Mellon University, USA)
"Development of atom transfer radical polymerization (ATRP)"
Prof. Mitsuo Sawamoto (Professor at Kyoto University, Japan)
"Precision polymerization and precision synthesis of functional polymers"

2015   **Prof. Harald Rose** (Professor at the University of Ulm, Germany)
Prof. Maximilian Haider (Professor at Karlsruhe Institute for Technology / Cofunder of the Corrected Electron Optical Systems GmbH, Germany)
Prof. Knut Wolf Urban (Professor, Research Centre Juelich, Germany)
"Theoretical study, development and popularization of the aberration corrector for electron microscopes, and its application to materials science"

2016   **Dr. Koichi Mizushima** (Executive Fellow, Toshiba Research Consulting Corporation, Japan)
Dr. Akira Yoshino (Adviser for Asahi Kasei Corporation/President at the Lithium Ion Battery Technology and Evaluation Center/Visiting Professor at the Research and Education Center for Advanced Energy Materials, Devices, and Systems, Kyushu University, Japan)
"Discovery of anode material for the lithium ion battery ($LiCoO_2$) and development of the lithium ion battery"

2017   **Prof. John Ågren** (Professor at the Royal Institute of Technology, Sweden)
"Development of kinetic simulation packages for computational thermodynamics"
Prof. Bo Sundman (Professor at the Royal Institute of Technology, Sweden)
"Development of thermodynamic calculation packages for computational thermodynamics"
Prof. Kiyohito Ishida (Professor Emeritus at Tohoku University, Japan)
"Alloy design and development of structural materials based on thermodynamics of phase diagrams and microstructures"

2018   **Dr. Masato Sagawa** (Advisor for Daido Steel Co., Ltd)
"Invention and practical application of neodymium magnets"
Prof. Terunobu Miyazaki (Professor Emeritus, Tohoku University)
"Development of tunneling magnetoresistance elements capable of generating giant magnetoresistance at room temperature and application thereof to spintronics devices"

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