

## EDITORIAL

Dear colleagues:

It is my pleasure to announce a special issue of the journal *POWDER DIFFRACTION* on “Crystallography and properties of metal organic framework (MOF) compounds”. The guest editors are Drs. Craig M. Brown and Winnie Wong-Ng, both from National Institute of Standards and Technology. The details of the CALL FOR PAPERS is described below.

*POWDER DIFFRACTION* (PDJ) is a quarterly journal published by the JCPDS-International Centre for Diffraction Data through the Cambridge University Press. *POWDER DIFFRACTION* is a journal of practical technique, publishing

articles relating to the widest range of application—from materials analysis to epitaxial growth of thin films and to the latest advances in software.

This special issue of PDJ will be open access for one year after the volume is published.

Camden R. Hubbard  
*Editor-in-Chief,*  
*Powder Diffraction*

## CALL FOR PAPERS

### Crystallography and properties of metal organic framework (MOF) compounds

Research on metal-organic framework (MOF) materials has been a fast-growing field over the past decade. The interest and excitement in these materials are evidenced by the explosion in the number of papers in the scientific literature with MOF-related papers among the most highly cited in recent years. The increasing attention is partly owing to the wide potential applications, including gas sorption, gas storage, gas separation, catalysis, sensors, drug delivery, imaging, electronic devices, and environmental sustainability. The development and fundamental understanding of the properties of MOF materials are therefore important to technological needs, and are at the forefront of materials research.

Crystallography provides the foundation of structure-property relationships. It bridges the fundamental understanding of materials with their applications. As functional MOF materials are envisioned to play an important role in our modern society and future economic and social success, the underlying crystallographic information for these materials is of utmost importance for many research communities.

While there have been a large number of papers dealing with structures of MOFs in many high-ranking journals, there has not been a focused effort that highlights the current state-of-the-art capabilities developed for university laboratory use or available at large-scale user facilities that allow materials to be probed *in-situ*, *in-operando*, or multiplexed with other analytical techniques. Therefore, this proposed special issue of Powder Diffraction will provide an important venue for authors and readers to recognize and appreciate the impact of these capabilities in understanding the structural implications on the function of MOFs. The guest editors anticipate that this anthology will serve the community as *the* reference for modern measurement capabilities, data analysis, and materials insight.

The goal of this special issue is to focus on the latest developments in the cross-disciplinary fields of structure science and MOF materials. Progress in measurement capabilities with *in situ*, *in operando*, multi-modal, and high-pressure crystallographic techniques are important areas for this issue to address. The types of materials of interest include bulk powders, single crystals, amorphous solids, thin films, and nanostructures. The

special issue will encompass up-to-date research topics of MOFs as well as with reviews that present new evaluation and analyses of published work. All the papers in the issue will be original with suggested topics listed here.

- Structure/property relationships
- Properties of interest: catalytic, sorption, mechanical, gas storage, separations, energy harvesting, sensing, luminescence, energy conversion, electrical, ion conductivity, and magnetic properties
- Scattering techniques:
  - Ambient X-ray (laboratory and synchrotron), neutron, and electron
  - *In situ*, *in operando* and non-ambient crystallography
- Software tools for the analysis of MOFs
- Instrumentation/techniques (combined use/multimodal) for analysis of MOFs
- Powders, single crystals, nanomaterials, thin films
- New materials and new crystallographic data
- Crystallography and computational modeling
- Nomenclature, terminology, classification scheme
- Industrial applications
- Vision/projection of MOFs in the coming years

The guest editors estimate each contributed paper to be between 5–8 printed pages. The papers will be either original reports of research work or an original review presenting the author’s own evaluation and analysis of recent research work and a future outlook.

### Timeline of Publication:

Manuscript submission:	June 30, 2018
Peer & Editor Reviews completed:	August 15, 2018
Final submission of revisions:	November 1, 2018
Journal standards revisions/acceptance	December 1, 2018
Publication date:	March 1, 2019

Note: Papers accepted for publication are made available online via First View shortly after author proof final acceptance following the Journal standards review & revisions.

## Guidelines for Authors

Please visit <http://www.icdd.com/resources/pdj/authors.htm> for details, and email the guest editors for questions concerning manuscript ideas/suitability.

## Submission of papers

Authors are requested to submit their manuscripts directly to the publisher online at <http://mc.manuscriptcentral.com/pdj>. See the instructions on submitting a manuscript linked on that page.

**Dr. Craig M. Brown** ([craig.brown@nist.gov](mailto:craig.brown@nist.gov)) received his B. A. Degree in Natural Science from Cambridge University, UK, in 1995. He obtained his D. Phil from the University of Sussex, UK, in the group of Prof. Kosmas Prassides in 1999 while resident at the Institute Laue-Langevin, Grenoble, France, in the high-resolution time-of-flight neutron spectroscopy group headed by Jose Dianoux. In 1999, he moved to the University of Maryland to be a Research Associate and an Instrument Scientist at the NIST Center for Neutron Research (NCNR). In 2005, he became a Staff Scientist at the Indiana University Cyclotron Facility while performing instrument scientist duties at the NCNR. He is currently an Affiliated Assistant Professor in the Chemical Engineering Department at the University of Delaware and a staff chemist at the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) where he leads the Structure and Dynamics of Materials Team that supports a suite of neutron instruments. His research interests are broad but center around the structural and dynamical characterizations of energy- and energy efficiency-related materials with over 80 publications in this field which are cited over 6400 times. His work has been recognized within the Federal Government with a Presidential Early Career Award for Scientists and Engineers (PECASE), a Department of Commerce Silver Medal, and most recently the 2016 NIST Samuel Wesley Stratton Award recognizing an unusually significant research contribution to science or engineering. Externally, he has been awarded a Neutron Scattering Society of America Science Prize, an Arthur S. Flemming Award, and was co-awarded the 2016 DOE Hydrogen and

Fuel Cells Program R&D Award for “outstanding achievements in absorbent-based hydrogen storage material research characterization” with J.R. Long from University of California, Berkeley.

**Dr. Winnie Wong-Ng** ([winnie.wong-ng@nist.gov](mailto:winnie.wong-ng@nist.gov)) received a B.Sc. degree in Chemistry from the Chinese University of Hong Kong, a PhD degree in Inorganic Chemistry from Louisiana State University, followed by post-doctoral and research associate/lecturer appointments in the Chemistry Department of University of Toronto, Canada. She worked for ICDD for several years as a critical review scientist. She joined the Ceramics Division of NIST as a staff chemist in 1988, where she is currently employed. Her main research areas at NIST included measurements and standards of technologically important materials in bulk and film forms. Her research has focused on the phase equilibria, X-ray crystallography, and crystal chemistry of functional materials. Currently, she is the co-leader of the project “Measurements, Standards, and Data for Energy Conversion Materials” in the Materials for Energy and Sustainable Development Group of NIST. She also works on a CO<sub>2</sub> Mitigation project. She is a distinguished fellow of ICDD, a fellow of American Association for the Advancement of Science (AAAS), American Crystallographic Association (ACA), and the American Ceramic Society (ACerS). She will be a new member of the 2018 World Academy of Ceramics (WAC). She received two Bronze Medals from the United States Department of Commerce (2002 and 2008), the 2004 McMurdie Award from ICDD, and the 2007 Spriggs Phase Equilibria Award from ACerS. She has over 340 publications and co-edited more than 25 books/proceedings. She served on the Board of Directors of ICDD (2010–2014), the past chair of the Electronics Division of the American Ceramic Society (2005–2006), and past president of NIST Association of Asian Pacific Americans (ANAPA, 2000–2003). She is an associate editor for Journal American Ceramic Society (2013-present), and the international report editor for Powder Diffraction (1999-present).

Craig M. Brown, Winnie Wong-Ng  
Guest Editors, *Powder Diffraction*