# Special Issue

## Recent Advances on X-ray Structure Determination and Refinement Procedures

## Message from the Guest Editor

In the year 2023, the 110th Anniversary of the first ever structure determination made by using an X-ray diffraction technique, a goal reached by sir William Henry Bragg (1862-1942) y sir William Lawrence Bragg (1890-1971), father and son respectively, is celebrated. Both the experimental advances represented by the Xray tubes designed by William David Coolidge (1873-1975) and the theoretical relationships between structure factors and atomic coordinates obtained by Arnold Johannes Wilhelm Sommerfeld (1868-1951), obtained both the very same year, were essential in order to accomplish this final objective. The main purpose of the current Special Issue is to present the widest and deepest possible view of the current research on X-ray structure determination and refinement procedures, including both single crystal and powder diffraction methodologies, either conventional or synchrotron, as well as computational methods and software development. Papers related to research applied to any aspect of the Materials Science area in its broadest sense are particularly well suited for this special issue.

## **Guest Editor**

Prof. Dr. Juan F. Van der Maelen

Department of Physical and Analytical Chemistry, University of Oviedo, Principality of Asturias, Oviedo, Spain

## Deadline for manuscript submissions

closed (31 December 2023)



an Open Access Journal by MDPI

Impact Factor 3.2
CiteScore 6.4
Indexed in PubMed



mdpi.com/si/156418

Materials
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
materials@mdpi.com

mdpi.com/journal/materials





an Open Access Journal by MDPI

Impact Factor 3.2 CiteScore 6.4 Indexed in PubMed





## About the Journal

## Message from the Editor-in-Chief

Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. Materials provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

#### Editor-in-Chief

Prof. Dr. Maryam Tabrizian

 Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
 Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

## **Author Benefits**

#### Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

## **High Visibility:**

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, Ei Compendex, CaPlus / SciFinder, Inspec, Astrophysics Data System, and other databases.

#### **Journal Rank:**

JCR - Q2 (Metallurgy and Metallurgical Engineering) / CiteScore - Q1 (Condensed Matter Physics)