

ICDD 2021 Spring Meetings - A Virtual Zoom Event

AGENDA

Synchrotron & Neutron Scattering Methods Subcommittee

Tuesday, 9 March 2021

9:00 am – 10:00 am EST

Robert Papoular, Chair

1. **Welcome Remarks** **R. Papoular**

2. **Appointment of Minutes Secretary** **Denise DelCasale**

3. **Approval of Minutes from [March 2019](#)**

4. **Review of Mission Statement**

The Synchrotron & Neutron Scattering Methods Subcommittee of the International Centre for Diffraction Data (ICDD) will connect the ICDD's Technical Committee with the international synchrotron and neutron scattering community. It will educate ICDD members about advances within the community, and help identify new opportunities to enhance ICDD databases. The subcommittee will provide recommendations to address unique aspects associated with these experimental methods, and will assist the technical staff of the ICDD to integrate information obtained at synchrotron and neutron scattering facilities into the ICDD databases.

5. **Board of Directors' Liaison Report** **V. Peterson**

Please note, in order for a motion to move forward, a task group (or leader) needs to be assigned and named within the motion. Vanessa will not be able to attend the meeting but has sent the following message:

"I have no information to report as board liaison. I will give a short member facility report: The Australian Centre for Neutron Scattering paused operations as a COVID response in April 2020, but recommenced work in July 2020. The Australian Synchrotron also ceased operations, recommenced in July 2020, and ceased operations for several months in November 2020 following a second outbreak in Victoria. Both facilities are currently fully operational, executing experiments remotely via a mail-in arrangements. As consistent with reports from elsewhere, there are additional overheads on staff for the execution of such experiments remotely, and many operations are affected substantially by shipping and the availability of samples. During 2020 the Australian Centre for Neutron Scattering began operating a second reflectometer, Spatz."

Best wishes,

Vanessa

Prof. Vanessa Peterson (FRSC FRACI CChem)

6. **TOF Developments in PDF-4** **S. Kabekkodu**

We continue to add calculated TOF entries with all the ICSD and LPF sourced new entries. There are no pending motions to act upon.

7. **Support for Importing 2D data into Sieve+ using the ESRF *.edf File Format** **J. Blanton**

8. A Novel Phasing Method Based on the Absolute Electron Density
(see attached abstract)

J. Rius

9. User Facility News

10. Magnetic contribution(s) to PDF entries?

11. New & Other Business

12. Adjournment

A Novel Phasing Method Based on the Absolute Electron Density

Jordi Rius

It is known that functions $\delta_M = FT^{-1}(E - \langle E \rangle) \cdot e^{i\varphi}$ and $\rho = FT^{-1}(E \cdot e^{i\varphi})$ can be regarded as proportional for intensity data reaching atomic resolution ^[1]. The discrepancy between both functions, given by $R_{M,|\rho|} = \int_V (\delta_M - k \cdot |\rho|)^2 dV$, can be expressed in exact form in terms of the $\Phi = \{\dots\varphi\dots\}$ phases of the structure factors and minimized through the recursive application of the so called $S_{M,|\rho|}$ algorithm which constitutes the essential part of the novel phasing method^[2]. The efficiency of $S_{M,|\rho|}$ will be discussed with test examples involving single-crystal data of crystal structures of different complexity including protein ones. The potential application of $S_{M,|\rho|}$ to powder diffraction data will be also shortly discussed. Since the novel method is very simple, has a strong theoretical basis and provides a more intuitive interpretation of the underlying functions, it is also ideal for teaching purposes.

[1] Rius, J. (2012) *Acta Cryst.* A68, 77-81

[2] Rius, J. (2020) *Acta Cryst.* A76, 489-493.