Electron Diffraction Subcommittee Meeting Minutes Wednesday, 13 March 2019 **International Centre Headquarters Conference Room D** 4:00 p.m. – 5:00 p.m. Alina Bruma, Chairman

- 1. Call to Order and Opening Remarks Attendance list on record at headquarters.
- 2. Appointment of Minutes Secretary J. Cannon was appointed to record minutes.
- 3. Approval of 2018 Minutes
 - Motion moved by:
 - All in agreement no official vote
- 4. Review of Mission Statement -

The Electron Diffraction Subcommittee serves as a bridge between the electron diffraction community and the other parts of ICDD. It will communicate the needs of electron diffraction specialists to ICDD, so that ICDD may more effectively respond to those needs. It will assist in communicating to the electron diffraction community the way in which ICDD will serve them. To these ends, it will cooperate with other ICDD subcommittees and with the central organization of ICDD. Specifically, the subcommittee shall monitor the status of and suggest improvements to the databases and related products used in electron diffraction (those produced by other organizations, as well as those produced by ICDD).

- 5. Board of Directors' Liaison Report (No motions or Report)
- 6. Marketing Sales Information Discussion
 - ICDD does not currently have an electron specific database. We are exploring what to do and \geq gathering feedback to determine the right way to proceed as far as software and the database itself
- 7. ED Software Suggested Updates:
 - > The Electron Diffraction task group evaluated the performance of electron diffraction sub-unit and offer suggestions for improvements of the database and test capability of the software regarding indexation electron diffraction patterns
 - Suggestions:
 - Smoother transition of the intensity of the electron diffraction spots
 - Include notations checkbox over spots for d spacing
 - Overlay the direction in the reciprocal lattice directly on the ED patterns.
 - ♦ Save in any graphic format
 - Transparent background not black
 - ♦ 3D model
 - Change atomic radius for atoms in the unit cell
 - Mask specific diffraction spots In reciprocal space-equivalent to centering Selected Area Diffraction aperture around specific diffraction spot
 - More restricted choice of structural information regarding compounds would be useful to have for fast screening
 - Addition of statistics: ie. the most frequently used data by other users or best pattern as alternative
 - User had problems indexing modular structures determine if this is a communication failure with the software or programming flaw (ICDD will create a tutorial to help with this)
 - Conclusions: \triangleright
 - First pilot test complete Software received well

M. Rodriguez

T. Blanton

A. Bruma

A. Bruma

A. Bruma

A. Bruma

- > Data (inorganic or organic, etc.) Need input from users
- > Atomic Coordinates Very important according to Alina
 - ◆If atomic coordinates are needed, ED database shouldn't be separate
 - ✤If atomic coordinates are not needed, ED database should be a separate database
- Further software suggestions and improvements from new group
- > Contact Justin for additional 10-15 task group members for coordination
- Possibility for Alina to attend M&M paid for by ICDD (Winnie believes OK), but will check with NIST for approval

9. Suggestions

- > Pilot a program with a larger number of researchers
- Timeline of implementation and prioritization of suggested changes for this release and next release

10. Adjournment

Motion moved by:

A. Bruma A. Bruma

A. Bruma

All in agreement – no official vote