

# Mini Workshop on ePDF, 28-29th of March 2018, Ulm, Germany

Building N27 of the Ulm University Campus

Albert-Einstein-Allee 11, 89081 Ulm, Germany



## Program

28<sup>th</sup> of March

|                                                                     |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
|---------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| 8:45-8:50                                                           | Tatiana Gorelik                                                                                                                                                                                                                                                                                             | Welcome                                                                                               |
| 8:50-9:10                                                           | Johannes Biskupek                                                                                                                                                                                                                                                                                           | TEM in Ulm, SALVE                                                                                     |
| <b>Applications</b>                                                 |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| 9:10-9:40                                                           | Viktoria Kovács Kis                                                                                                                                                                                                                                                                                         | Mineralogical applications                                                                            |
| 9:40-10:10                                                          | Konstantin Borisenko                                                                                                                                                                                                                                                                                        | Current work on electron PDF in Oxford                                                                |
| 10:10-10:40                                                         | Partha Das                                                                                                                                                                                                                                                                                                  | Structural analysis of amorphous & nano-crystalline materials by electron diffraction PDF             |
| <i>10:40-11:00 Coffee Break</i>                                     |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| <b>Software</b>                                                     |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| 11:00-11:20                                                         | Alejandro Gomez Perez                                                                                                                                                                                                                                                                                       | DEMO: ePDF suite                                                                                      |
| 11:20-12:00                                                         | Cheuk-Wai Tai                                                                                                                                                                                                                                                                                               | SUePDF – electron diffraction data to PDF, DEMO                                                       |
| 12:00-12:40                                                         | Janos Labar                                                                                                                                                                                                                                                                                                 | Introduction to Process Diffraction, DEMO                                                             |
| <i>12:40-14:00 Lunch, we will install and try the programs here</i> |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| <b>Special topics</b>                                               |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| 14:00-14:20                                                         | Xiaoke Mu                                                                                                                                                                                                                                                                                                   | Radial distribution function imaging by 4DSTEM and association with multivariate statistical analysis |
| 14:20-14:40                                                         | Christopher Wright                                                                                                                                                                                                                                                                                          | Algorithms and approaches for robust PDFs                                                             |
| 14:40-15:00                                                         | Tatiana Gorelik                                                                                                                                                                                                                                                                                             | Elastic / inelastic diffraction                                                                       |
| 15:00-15:30                                                         | Reinhard Neder, Tatiana Gorelik                                                                                                                                                                                                                                                                             | Preferred orientation / texture in PDF                                                                |
| <i>15:30-16:00 Coffee Break</i>                                     |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| <b>Interactive session - Discussions</b>                            |                                                                                                                                                                                                                                                                                                             |                                                                                                       |
| 16:00-18:00                                                         | Propagation of data centering errors in PDF; Resolution in PDF and PDF images; Artefacts in PDF; Multiple scattering; Comparing detectors PDF, effect of the recording medium – point spread function, etc.; Distortion of diffraction patters; Background treatment; Instrumental influence in PDF; etc... |                                                                                                       |
| <i>19:30 – Dinner in Hacker-Pschorr (Sterngasse 17)</i>             |                                                                                                                                                                                                                                                                                                             |                                                                                                       |

29<sup>th</sup> of March

| <b><i>Quantitative interpretation of ePDF</i></b> |                 |                                         |
|---------------------------------------------------|-----------------|-----------------------------------------|
| 8:30-9:00                                         | Reinhard Neder  | ePDF refinement                         |
| 9:00-10:00                                        | Reinhard Neder  | DISCUS DEMO: PDF simulation, refinement |
| <i>10:00-10:30 Coffee Break</i>                   |                 |                                         |
| 10:30-11:45                                       |                 | <i>Try programs with your own data</i>  |
| 11:45-12:00                                       | Tatiana Gorelik | Concluding remarks                      |
| <i>12:00-13:30 Lunch, departure</i>               |                 |                                         |

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