Report on the 1. International Charge Density Meeting (ICDM 2019)

21. – 26. July 2019 at the Georg-August-Universität Göttingen

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The 1. ICDM 2019 was launched at the conference venue Alte Mensa in the historic city centre of Göttingen. The meeting succeeded the established European Charge Density Meeting ECDM 7 in Warsaw, held in 2016 by our colleague Krzysztof Woszniak. It was then when the steering comity decided to open the European format (maintained since the beginning in 1996 in Nancy) to our international colleagues, counterbalancing the loss of the Charge, Spin and Momentum Density Gordon Research Conference.

All participants were accommodated in hotels within walking distance to the conference site. In total we hosted 102 delegates (26 ♀ / 76 ♂), 47 from Germany and 55 from world-wide. In addition to the attendees from most European countries we had participants from Australia, India, Japan, Mexico, Russia, South Africa, and the United States of America. The speakers were suggested, selected and confirmed with the help of the scientific advisory board. At this point I want to thank Carlo Gatti, Milano; Simon Grabowsky, Bremen; John R. Helliwell, Manchester; Sine Larsen, Copenhagen; Claude Lecomte, Nancy; Piero Macchi, Bern; Chérif F. Matta, Halifax; Alan Pinkerton, Toledo, Ohio; Guru T. Row, Bangalore; Wolfgang Scherer, Augsburg; Sander van Smaalen, Bayreuth; and Krzysztof Woźniak, Warsaw, for their constant help and advice. The program was scheduled into 41 slots of 30 min. talks, clustered to overarching topics. In addition to the talks we had 35 posters (13 ♀ / 22 ♂) on constant display during the conference with one specially dedicated 2 ½ hours slot on Tuesday afternoon.

The scientific program covered all aspects of contemporary modern charge density determination, spanning from experiment to theory, from molecules to materials chemistry, from time-resolved methods to NMR spectroscopy. All of the most dynamic and rapidly developing topics in science like *data and model quality*, *non-covalent interactions*, *materials profiles from charge density*, *charge density in life science*, *non-ambient conditions*, *computational methods*, *Why measure, just compute!*, *New technologies*, *dynamics*, *and NMR and charge density* were addressed by several contributions. At the end of each talk there was designated time for questions and remarks, followed by lively discussions in the coffee breaks. Young scientists could easily approach the high profilers, either challenging them or asking for advice in discussions, frequently in front of their posters.

In this format there certainly is neither room for nor need to summarize the whole conference, so I will spotlight only a few of the contributions, which all were of remarkable high interest and quality.

The conference started with *data and model quality*. Obviously, the field experiences currently a remarkable burst in experimental as well as in computational progress. Spring-8 in Japan and Petra-III are the world's leading large facilities in diffraction with a remarkable power and coherence, enabling charge density investigations even from powder samples. Eiji Nishibori from the University of Tsukuba in Japan started the conference and reported on a charge density study from aluminium and diamond with Spring-8 X-ray powder diffraction techniques to reveal weak interactions in those materials. They are of vital interest to scale structure to property profile. Any experimental data require structure modelling software. The author of the program MoPro, Christian Jelsch from the University de Lorraine at Nancy, reported of benchmarking the modelling exemplified at the drug aceclofenac, a most important non-steroidal anti-inflammatory, widely used in the medication of mitigate pain and inflammation.

The next slot of eight speakers was dedicated to *non-covalent interactions*. Just limited to hydrogen bonding for long, today there is an entire new set of NCIs identified to coin materials profiles. Yuri Grin

from Dresden talked about the ELI/ED approach that facilitates differentiation of covalent and ionic contributions in intermetallic chlatrates. With the new tools the formation of the lone pairs around the defects in the covalently bonded framework can be revealed, obviously responsible for unusual thermal transport in these thermoelectrics. Sajesh Thomas, currently at the University of Aarhus, reported on one of the most underexplored features of intermolecular non-covalent interactions, the electric field exerted by molecules on their nearest neighbours. Among others, he presented insights from the charge density analyses of a series of crystalline host-guest systems using combined X-ray and neutron diffraction where he not only investigated the local electric fields, but also their effect on intramolecular bonds – manifested as vibrational frequency shifts. Erna Wieduwilt from the University de Lorraine at Metz, brought NCI-ELMO, a new computational method to extract non-covalent interactions in systems of biological interest, to the attention of the audience.

Jacob Overgaard from the University of Aarhus started the session on *materials profiles from charge density* by elucidating the mechanisms of single molecule magnets (SMMs) using diffraction methods. He showed how charge density studies of two dysprosium SMMs experimentally confirmed the predicted oblate shape of the valence density while also indicating the mixed composition of the ground state. Furthermore, he used polarized neutron single crystal data and provided quantitative knowledge of the local susceptibility tensor in SMMs. In his talk the Grand Seigneur of charge density, Carlo Gatti from Milano, appealed to try to export and sell Quantum Crystallography knowledge in domains where it might be useful but where it is instead yet poorly known. He discussed as exemplary first chalcogenide phase-change materials, second the enantioseparation outcome in the HPLC environment, and third the empirical links between bond indicators and Bond Valence (BV) parameters of Pauling's BV method.

In the session concerning *charge density in life science* Paulina Dominiak from the University of Warsaw talked about shifting from electron density to electrostatic potential perspectives. Electron density and electrostatic potential are the key properties of molecules and their assemblies. Many other chemically or biologically relevant properties originate from them. News from interfacing their new software library DiSCaMB with Olex2 where reported. Results of Transferable Aspherical Atom Model refinements on a large data set clearly showed advantages and disadvantages in comparison to the Independent Atom Model and Hirshfeld Atom Refinement.

Computational methods where introduced by Ángel Pendás from the University of Oviedo. He dealt with a chemical fragment as a truly open quantum system. Using techniques borrowed from the theory of open quantum systems, he showed how the partial trace over the environment degrees of freedom can be defined in real space. José E. Barquera-Lozada from UNAM, Mexico, showed that the direction of the rotation of the vectorial field induced current density can be compressed in the scalar field. This has similarities with the Laplacian of the electron density but contrary to the Laplacian, it can easily distinguish between main-group aromatic and antiaromatic molecules.

The Wednesday morning session was opened by *NMR* and the talks of Christian Griesinger from the MPI of biophysical chemistry, Göttingen, and Ann-Christin Pöppler from the University of Würzburg. The latter spoke of structural models of polymer micelles using solid-state NMR, powder X-ray diffraction and calculations.

High-pressure work from Piero Macchi, Milano, started the *non-ambient conditions* session. He presented the electron density and dielectric properties of highly porous MOFs in respect to binding and mobility of guest molecules in Cu_3- and Zn_3(1,3,5-benzenetricarboxylate)$_2$. Roman Gajda from the University of Warsaw talked about the experimental charge density study of grossular ($Ca_3Al_2Si_3O_{12}$) under pressure and compared it to pyrop ($Mg_3Al_2Si_3O_{12}$).

The Thursday morning was covered by vendor talks from Rigaku, Excillum, Dectris, Incoatec and Bruker, presenting their latest developments. The afternoon was dedicated to the provocative statement *Why measure, just compute!* Paul Popelier from the University of Manchester started with Interacting

Quantum Atoms (IQA) and the Relative Energy Gradient (REG) method and how to extract chemical insight from wave functions. The latter is able to explain the gauche effect, the torsional barrier in biphenyl, the peptide hydrolysis in the HIV-1 protease active site), halogenalkane nucleophilic substitution (SN_2) reactions and the factors controlling the nature of complementary hydrogen-bonded networks as found in nucleic acid base pairs. Alessandro Genoni from the University de Lorraine at Metz presented the first HAR-ELMO refinements of polypeptides (e.g., Leu-enkephalin, fibril-forming segment of the human prion protein) and proteins (e.g., crambin), illustrating possible ways to further improve their proposed technique.

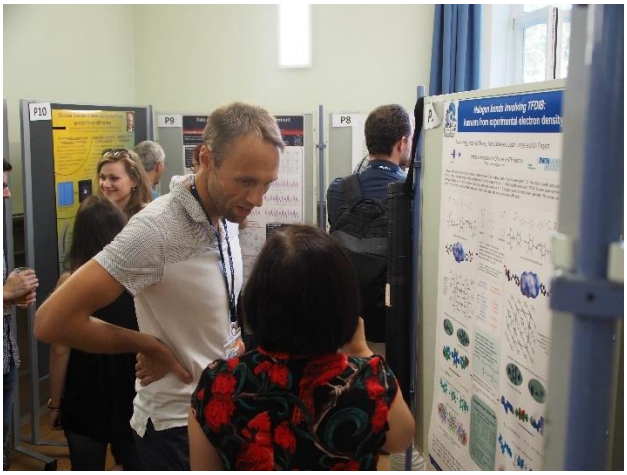
The session *dynamic quantum crystallography* was defrayed by Thomas Elsaesser from the Max-Born-Institute of non-linear optics in Berlin and Anders Madsen from the University of Kopenhagen. The first spoke about transient charge density in polar crystals from femtosecond X-ray diffraction. In polar and/or ionic crystals, Coulomb interactions mediated via local electric fields play a central role in coupling electronic and nuclear motions. Femtosecond x-ray diffraction allows for following such correlated dynamics at the atomic level by providing momentary atom positions and charge density distributions. Anders Madsen is devoted to nuclear motion in correlation to electron density. He votes for the amalgamation into a common model, which can be compared and refined against the experimental evidence, and which can be used to understand solid state properties at the atomic level.

The last topic of the meeting were *new technologies*. Lennard Krause, currently at Aarhus University, identified two obstacles in the measuring of accurate single crystal diffraction data using a Pilatus3 CdTe detector: First, too low intensities for weak reflections, originating from the data processing, specifically in the outlier rejection and data averaging. Second, disregarding charge sharing between pixels within strong reflections leads to unreasonably large extinction parameters.

From the rich and top-class variety of contributed posters a jury picked three to be awarded as the best posters of the conference. One was presented by Benjamin De Bruyne from CentraleSupélec, Gif-sur-Yvette, France, entitled to inferring a 1-RDM for molecular crystals from expectation values under N-representability conditions. The method has been applied to the crystal of dry ice. A one-electron reduced density matrix of reference has been obtained by periodic ab-initio calculations. The next poster was presented by Max Davidson from the University of Western Australia, Perth. The poster devoted to fragHAR: towards *ab initio* quantum crystallographic X-ray structure refinement for polypeptides and proteins was granted with the Robert Farrell Stewart Award to commemorate a giant in charge density investigation. The third prize went to Sylwia Pawlędzio. She presented her work on data processing and Hirshfeld atom refinement of a organo-gold(I) complex. The results from DFT-based refinements with the nonrelativistic (NR) and quasi-relativistic (IOTC) approaches were compared.

The meeting was closed by a confident resume and perspective outlook of Jean-Michel Gillet from CentraleSupélec, Gif-sur-Yvette, France. As venue for the next ICDM Denmark with the Universities of Aarhus and Copenhagen was admittedly established.

The Conference Picture



Poster Discussions

Poster Prizes

Conference Dinner

Conference Excursion to the world heritage Bergpark Wihelmshöhe in Kassel

Overall, we had a most enjoyable and fruitful conference, witnessing that international exchange across political borders in a relaxed atmosphere is indispensable important. The connections initiated at this conference especially amongst young scientists will last. Those between the established colleagues have been broadened and fostered, proving that the ICDM is a most valuable format that should be continuously supported and financed.

Göttingen, 23.03.2020

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