

Stef Smeets

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Research Experience

- Jan 2016–Now **Postdoc**, *Inorganic and Structural Chemistry, Stockholm University, SE*.
Developed methodology to collect and process serial electron diffraction data, developed electron diffraction data collection software, analysed zeolite crystal structures. Advisor: Dr. Wei Wan.
- Nov 2011–
Dec 2015 **Research assistant**, *Lab. for Crystallography, ETH Zurich, CH*.
Developed approaches to combine computational and experimental methods for structure determination of polycrystalline materials, determined and refined the crystal structures of zeolites against X-ray powder diffraction data. Advisor: Dr. L.B. McCusker.
- May 2014 **Visiting student**, *Inorganic and Structural Chemistry, Stockholm University, SE*.
Visited the group of Prof. X. Zou to collect electron diffraction data.
- Feb–Jul 2011 **Intern**, *Chemical Crystallography, University of Zaragoza, ES*.
Developed software to analyse thermal atomic motion of a crystalline transition metal complexes). Advisor: Prof. L.R. Falvello.
- Feb–Dec 2010 **Master student**, *Crystal and Structural Chemistry, Utrecht University, NL*.
Analysed the temperature-dependence of the crystal structure, thermal motion, and disorder of transition metal complexes. Advisor: Dr. M. Lutz.
- Apr–Jun 2009 **Bachelor student**, *Crystal and Structural Chemistry, Utrecht University, NL*.
Analysed the temperature-dependence of organic crystal structures. Advisor: Dr. M. Lutz.

Education

- Nov 2015 **PhD in Materials Science**, *ETH Zurich, CH*.
Thesis title: Development of hybrid methods for solving the structures of polycrystalline materials.
- Aug 2011 **MSc in Chemical Sciences**, *Utrecht University, NL*, GPA: 4.00/4.
- Jul 2009 **BSc in Chemical Sciences**, *Utrecht University, NL*, GPA: 3.05/4.
- Jul 2004 **International Baccalaureate**, *International School Hilversum, NL*.

Awards and fellowships

- 2018 Awarded [EPDIC Award for Young Scientists](#) for outstanding scientific achievement in the field of powder diffraction
- 2017 One-year [SNF Advanced Postdoc.Mobility fellowship](#) for development of serial electron crystallography methods for quantitative phase analysis
- 2017 Awarded [7th FEZA PhD prize](#) for the highest quality zeolite-related publications arising from PhD research
- 2017 Awarded [Swiss Society for Crystallography PhD prize](#) for the best thesis in crystallography
- 2016 Awarded [ETH Medal](#) for outstanding doctoral thesis (top 8%)
- 2015 Two-year [SNF Early Postdoc.Mobility fellowship](#) for development of serial electron crystallography methods for structure determination of beam-sensitive materials

Publications

- 2018 **S. Smeets***, W. Wan, and X. Zou, Serial Electron Crystallography for Structure Determination and Phase Analysis of Nanocrystalline Materials, *J. Appl. Crystallogr.*, Accepted for publication, **2018**
- P. Rzepka, D. Wardecki, **S. Smeets**, M. Müller, H. Gies, X. Zou, and N. Hedin, CO₂-induced displacement of Na⁺ and K⁺ in zeolite [NaK]-A, *J. Phys. Chem. C*, doi: 10.1021/acs.jpcc.8b03899, **2018**
 - M.O. Cichocka, Y. Lorgouilloux, **S. Smeets**, J. Su, W. Wan, P. Caullet, N. Bats, L.B. McCusker, J.-L. Paillaud, and X. Zou, Multidimensional Disorder in Zeolite IM-18 Revealed by Combining Transmission Electron Microscopy and X-ray Powder Diffraction Analyses, *Cryst. Growth Des.* 18(4):2441-2451, **2018**
- 2017 Y. Luo, **S. Smeets**, F. Peng, A.S. Etman, Z. Wang, J. Sun, and W. Yang, Synthesis and Structure Determination of Large-Pore Zeolite SCM-14, *Chem. Eur. J.* 23(66):16829-16834, **2017**
- **S. Smeets***, Z.J. Berkson, D. Xie, S.I. Zones, W. Wan, X. Zou, M.-F. Hsieh, B.F. Chmelka, L.B. McCusker, and C. Baerlocher, Well-Defined Silanols in the Structure of the Calcined High-Silica Zeolite SSZ-70: New Understanding of a Successful Catalytic Material, *J. Am. Chem. Soc.* 139(46):16803-16812, **2017**
 - **S. Smeets***, and L.B. McCusker, Location of Organic Structure-Directing Agents in Zeolites Using Diffraction Techniques in *Structure and Bonding: New Insights into the Chemistry of Organic Templating in the Synthesis of Zeolitic Materials*, 1-31, **2017**
 - **S. Smeets**, and X. Zou, Zeolite Structures in *Zeolites in Catalysis: Properties and Applications*, 37-72, **2017**
 - **S. Smeets***, and W. Wan, Serial electron crystallography: merging diffraction data through rank aggregation, *J. Appl. Crystallogr.* 50(3):885-892, **2017**
- 2016 J.H. Kang, D. Xie, S.I. Zones, **S. Smeets**, L.B. McCusker, and M.E. Davis, Synthesis and Characterization of CIT-13, a Germanosilicate Molecular Sieve with Extra-Large Pore Openings, *Chem. Mater.* 28(17):6250-6259, **2016**
- **S. Smeets**, L.B. McCusker, C. Baerlocher, S. Elomari, D. Xie, and S.I. Zones, Locating Organic Guests in Inorganic Host Materials from X-ray Powder Diffraction Data, *J. Am. Chem. Soc.* 138(22):7099-7106, **2016**
- 2015 **S. Smeets**, L. Liu, J. Dong, and L.B. McCusker, Ionothermal Synthesis and Structure of a New Layered Zirconium Phosphate, *Inorg. Chem.* 54(16):7953-7958, **2015**
- **S. Smeets**, L. Koch, N. Mascello, J. Sesseg, L.B. McCusker, M. Hernández-Rodríguez, S. Mitchell, and J. Pérez-Ramírez, Structure analysis of a BEC-type germanosilicate zeolite including the location of the flexible organic cations in the channels, *CrystEngComm* 17(26):4865-4870, **2015**
 - C. Dejoie, **S. Smeets**, C. Baerlocher, N. Tamura, P. Pattison, R. Abela, and L.B. McCusker, Serial snapshot crystallography for materials science with SwissFEL, *IUCrJ* 2(3):361-370, **2015**
 - **S. Smeets**, L.B. McCusker, C. Baerlocher, D. Xie, C.-Y. Chen, and S.I. Zones, SSZ-87: A Borosilicate Zeolite with Unusually Flexible 10-Ring Pore Openings, *J. Am. Chem. Soc.* 137(5):2015-2020, **2015**

- 2014 **S. Smeets**, D. Xie, C. Baerlocher, L.B. McCusker, W. Wan, X. Zou, and S.I. Zones, [High-Silica Zeolite SSZ-61 with Dumbbell-Shaped Extra-Large-Pore Channels](#), *Angew. Chem.* 126(39):10566-10570, **2014**
- **S. Smeets**, D. Xie, L.B. McCusker, C. Baerlocher, S.I. Zones, J.A. Thompson, H.S. Lacheen, and H.-M. Huang, [SSZ-45: A High-Silica Zeolite with Small Pore Openings, Large Cavities, and Unusual Adsorption Properties](#), *Chem. Mater.* 26(13):3909-3913, **2014**
 - G. Majano, O. Martin, M. Hammes, **S. Smeets**, C. Baerlocher, and J. Pérez-Ramírez, [Solvent-Mediated Reconstruction of the Metal–Organic Framework HKUST-1 \(Cu₃\(BTC\)₂\)](#), *Adv. Funct. Mater.* 24(25):3855-3865, **2014**
 - T.R. Amarante, P. Neves, A.C. Gomes, M.M. Nolasco, P. Ribeiro-Claro, A.C. Coelho, A.A. Valente, F.A.A. Paz, **S. Smeets**, L.B. McCusker, M. Pillinger, and I.S. Gonçalves, [Synthesis, Structural Elucidation, and Catalytic Properties in Olefin Epoxidation of the Polymeric Hybrid Material \[Mo₃O₉\(2-\[3\(5\)-Pyrazolyl\]pyridine\)\]_n](#), *Inorg. Chem.* 53(5):2652-2665, **2014**
- 2013 R. Chen, J. Yao, Q. Gu, **S. Smeets**, C. Baerlocher, H. Gu, D. Zhu, W. Morris, O.M. Yaghi, and H. Wang, [A two-dimensional zeolitic imidazolate framework with a cushion-shaped cavity for CO₂ adsorption](#), *Chem. Commun.* 49(82):9500-9502, **2013**
- **S. Smeets**, L.B. McCusker, C. Baerlocher, E. Mugnaioli, and U. Kolb, [Using FOCUS to solve zeolite structures from three-dimensional electron diffraction data](#), *J. Appl. Crystallogr.* 46(4):1017-1023, **2013**
- 2011 **S. Smeets**, and M. Lutz, [Hexakis\(urea-kO\)zinc\(II\) dinitrate at 110 and 250 K: uniaxial negative thermal expansion](#), *Acta Cryst. C* 67(2):m50-m55, **2011**
- **S. Smeets**, P. Parois, H.-B. Bürgi, and M. Lutz, [Temperature-dependent analysis of thermal motion, disorder and structures of tris\(ethylenediamine\)zinc\(II\) sulfate and tris\(ethylenediamine\)copper\(II\) sulfate](#), *Acta Cryst. B* 67(1):53-62, **2011**
- 2010 M. Lutz, **S. Smeets**, and P. Parois, [catena-Poly\[\[bis\(ethylenediamine\)copper\(II\)\]-u-sulfato\]](#), *Acta Cryst. E* 66(6):m671-m672, **2010**

Conference talks

- 2018 **Invited oral presentation**: Zeolite SSZ-70: new understanding of a successful catalytic material, [ECM-31](#), Oviedo, ES, 22-27 August
- **Plenary lecture**: Structure determination of polycrystalline materials using X-rays and electrons, [EPDIC-16](#), Edinburgh, UK, 1-4 July
- 2017 **Invited oral presentation**: Serial electron diffraction for phase analysis and structure determination of polycrystalline materials, [NVK-2017](#), Oss, NL, 3 Nov
- **Invited oral presentation**: Structure analysis of polycrystalline materials using X-rays and electrons, [SGK-2017](#), Geneva, CH, 12 Sep
 - **Oral presentation**: Serial electron diffraction for phase analysis and structure determination, [IUCr2017](#), Hyderabad, IN, 21 to 28 Aug
 - **Invited oral presentation**: Characterization of zeolite structures using X-ray powder diffraction: framework structures, heteroatoms, and structure-directing agents, [FEZA2017](#), Sofia, BA, 3 to 7 Jul

- **Oral presentation:** The structure of zeolite SSZ-70 through combined HRTEM, XRPD, and DNP-enhanced 2D NMR, [Inorganic days](#), Nynäshamn, SE, 12 to 14 Jun
- 2016 **Oral presentation:** Serial snapshot crystallography using electron diffraction, [ECM-30](#), Basel, CH, 28 Aug to 1 Sep
- 2015 **Oral presentation:** Indexing of multi-crystal snapshots collected with a broad bandpass beam, [ECM-29](#), Rovinj, HR, 23 to 28 Aug
 - **Oral Presentation:** How do the positions of organic structure-directing agents determined from powder diffraction data compare with those from molecular modelling? [BZA-38](#), Chester, UK, 26 to 31 Jul
- 2014 **Invited oral presentation:** When two bad data sets are better than one, [IUCr2014](#), Montreal, CA, 5 to 12 Aug ([abstract](#); received travel support)
 - **Invited oral presentation:** Difficult structures come in a variety of flavors, [EPDIC-14](#), Aarhus, DK, 15 to 18 Jun
- 2013 **Oral presentation:** Using FOCUS and Superflip to solve structures from 3D electron and powder diffraction data, [ECM-28](#), Warwick, UK, 25 to 29 Aug ([abstract](#))