

# KRISTJAN EIMRE

## CURRICULUM VITAE

### PERSONAL DATA

**e-mail** [kristjaneimre@gmail.com](mailto:kristjaneimre@gmail.com)  
**website** <https://kristjaneimre.eu>  
**GitHub** <https://github.com/eimrek>  
**languages** English, Estonian

### EDUCATION

- 2017 – 2022 **Ph.D. in Materials Science**, Swiss Federal Laboratories for Materials Science and Technology (Empa) and University of Zurich  
*thesis*: [Engineering Novel Graphene-Based Nanostructures: A Computational Perspective](#)
- 2015 – 2017 **M.Sc. in Physics**, University of Tartu, *cum laude*  
*thesis*: [Multiscale electrical and thermal simulations of metal surface defects in high electric field](#)
- 2011 – 2015 **B.Sc. in Physics**, minor in Comp. Sci., University of Tartu, *cum laude*  
*thesis*: [Implementing the general thermal-field emission equation to the high electric field nanoprotrusion model](#)

### PROFESSIONAL EXPERIENCE

- 2022 – NOW **PostDoc/Research Software Engineer** at Swiss Federal Institute of Technology in Lausanne (EPFL), [Theory and Simulation of Materials group](#) (with Prof. Nicola Marzari, Dr. Giovanni Pizzi)
- Primary maintainer and developer of the [www.materialscloud.org](http://www.materialscloud.org) open science platform. (Technologies: React, FastAPI, Flask, MongoDB, ansible, OpenStack, Docker, Dokku)
  - Member of the [AiiDA](#) (Python) data and workflow infrastructure development team.
  - Contributing to science projects such as the [Materials Cloud 3D crystals database](#).
  - Contributing to the [OPTIMADE](#) ecosystem and integrating it with Materials Cloud.
  - Successful application for the Google Summer of Code and supervision of a student.
- 2017 – 2022 **Junior Researcher** at Swiss Federal Laboratories for Materials Science and Technology (Empa), [nanotech@surface laboratory](#) (with Prof. Roman Fasel, Dr. Carlo Pignedoli)
- Studying carbon nanomaterials with density functional theory (DFT) and beyond-DFT methods, in close collaboration with experiments.
  - Primary DFT software: CP2K, Quantum ESPRESSO, Gaussian, ORCA.
  - Co-authored over 25 scientific publications.
  - Built automation tools for computational tasks using [AiiDA](#); core contributor of the [AiiDALab](#) platform.
  - Set up and administered a local Linux compute machine with ~10 users.
  - Teaching assistant for courses: Statistical Mechanics and Molecular Simulations (Uni. Zurich), Condensed Matter Electronic Structure Theory (Uni. Zurich), Molecular and Materials Modelling (ETHZ). Supervised a Bachelor's thesis.
- 2014 – 2017 **Research Assistant** at University of Tartu, Intelligent Materials and Systems Lab (with Prof. A. Aabloo, Dr. V. Zadin)
- Studying metal surface defects in high electric fields to understand vacuum breakdown phenomena in particle accelerators. Used finite element (COMSOL), density functional theory (VASP) and quantum transport methods.
  - Co-authored 6 scientific publications.
  - Developed a C++ code to run finite element simulations (<https://github.com/eimrek/dealii-field-currents-heating>).
  - Teaching assistant for Computational Physics course.

- 2016 SUMMER **Intern** at Aalto University, Multiscale Statistical and Quantum Physics group (with Prof. T. Ala-Nissilä, Dr. V. Heinonen, Dr. C. V. Achim)
- Implementing and improving phase field crystal models. (report: <https://kristjaneimre.eu/c/pfc.pdf>)
  - Developed a C++ MPI code to perform phase field crystal modelling and benchmarked various optimization algorithms for the mechanical equilibration step (<https://github.com/eimrek/phase-field-crystal-mpi>).
- 2015 SUMMER **Intern** at the CMS collaboration, CERN (with Dr. S. Zelepoukine)
- Engineering project to build a hardware and software solution for temperature and humidity sensor calibration. (report: <https://cds.cern.ch/record/2046232>)

## PUBLICATIONS

\* denotes equally contributing first authors, † denotes corresponding authors

- 2024 **Jupyter Widgets and Extensions for Education and Research in Computational Physics and Chemistry**  
 Du, D.,\* Baird, T.J.,\* Eimre, K., Bonella, S., Pizzi, G.,† *Computer Physics Communications* 305, 109353. <https://doi.org/10.1016/j.cpc.2024.109353>
- Developments and Applications of the OPTIMADE API for Materials Discovery, Design, and Data Exchange**  
 Evans, M.L. et al., *Digital Discovery* 3, 1509–1533. <https://doi.org/10.1039/D4DD00039K>
- Electronic Decoupling and Hole-Doping of Graphene Nanoribbons on Metal Substrates by Chloride Intercalation**  
 Kinikar, A., Englmann, T.G., Di Giovannantonio, M.,† Bassi, N., Xiang, F., Stolz, S., Widmer, R., Borin Barin, G., Turco, E., Eimre, K., Merino Díez, N., Ortega-Guerrero, A., Feng, X., Gröning, O., Pignedoli, C.A.,† Fasel, R., Ruffieux, P.,† *ACS Nano* 18, 16622–16631. <https://doi.org/10.1021/acsnano.4c00484>
- Sterically Selective [3 + 3] Cycloaromatization in the On-Surface Synthesis of Nanographenes**  
 Kinikar, A., Wang, X., Di Giovannantonio, M., Urgel, J.I., Liu, P., Eimre, K., Pignedoli, C.A.,† Stolz, S., Bommert, M., Mishra, S., Sun, Q., Widmer, R., Qiu, Z., Narita, A., Müllen, K.,† Ruffieux, P., Fasel, R.,† *ACS Nanosci. Au* 4, 128–135. <https://doi.org/10.1021/acsnanoscienceau.3c00062>
- How to Verify the Precision of Density-Functional-Theory Implementations via Reproducible and Universal Workflows**  
 Bosoni, E. et al., *Nat Rev Phys* 6, 45–58. <https://doi.org/10.1038/s42254-023-00655-3>
- Tailoring Magnetism of Graphene Nanoflakes via Tip-Controlled Dehydrogenation**  
 Zhao, C.,\*† Huang, Q.,\* Valenta, L., Eimre, K., Yang, L., Yakutovich, A.V., Xu, W., Ma, J., Feng, X., Juriček, M., Fasel, R., Ruffieux, P.,† Pignedoli, C.A.,† *Phys. Rev. Lett.* 132, 046201. <https://doi.org/10.1103/PhysRevLett.132.046201>
- 2023 **On-Surface Interchain Coupling and Skeletal Rearrangement of Indenofluorene Polymers**  
 Chen, Q., Di Giovannantonio, M.,† Eimre, K., Urgel, J.I., Ruffieux, P., Pignedoli, C.A., Müllen, K., Fasel, R.,† Narita, A.,† *Macromolecular Chemistry and Physics* 224, 2300345. <https://doi.org/10.1002/macp.202300345>
- On-Surface Synthesis of Edge-Extended Zigzag Graphene Nanoribbons**  
 Kinikar, A., Xu, X., Giovannantonio, M.D., Gröning, O., Eimre, K., Pignedoli, C.A., Müllen, K., Narita, A.,† Ruffieux, P., Fasel, R.,† *Advanced Materials* 35, 2306311. <https://doi.org/10.1002/adma.202306311>
- Steering Large Magnetic Exchange Coupling in Nanographenes near the Closed-Shell to Open-Shell Transition**  
 Biswas, K.,\* Soler, D.,\* Mishra, S.,\* Chen, Q.,\* Yao, X.,\* Sánchez-Grande, A., Eimre, K., Mutombo, P., Martín-Fuentes, C., Lauwaet, K., Gallego, J.M., Ruffieux, P., Pignedoli, C.A., Müllen, K., Miranda, R., Urgel, J.I.,† Narita, A.,† Fasel, R.,† Jelínek, P.,† Écija, D.,† *J. Am. Chem. Soc.* 145, 2968–2974. <https://doi.org/10.1021/jacs.2c11431>

- 2022 **On-surface polyarylene synthesis by cycloaromatization of isopropyl substituents**  
Kinikar, A.,\* Di Giovannantonio, M.,\* Urgel, J.I., Eimre, K., Qiu, Z., Gu, Y., Jin, E., Narita, A., Wang, X.-Y., Müllen, K.,† Ruffieux, P., Pignedoli, C.A.,† Fasel, R.,† *Nat. Synth* 1, 289–296. <https://doi.org/10.1038/s44160-022-00032-5>
- On-surface synthesis and characterization of nitrogen-substituted undecacenes**  
Eimre, K.,\*† Urgel, J.I.,\*† Hayashi, H.,\* Di Giovannantonio, M., Ruffieux, P., Sato, S., Otomo, S., Chan, Y.S., Aratani, N., Passerone, D., Gröning, O., Yamada, H.†, Fasel, R.,† Pignedoli, C.A.,† *Nat Commun* 13, 511. <https://doi.org/10.1038/s41467-022-27961-1>
- 2021 **Observation of fractional edge excitations in nanographene spin chains**  
Mishra, S.,\* Catarina, G.,\* Wu, F., Ortiz, R., Jacob, D., Eimre, K., Ma, J., Pignedoli, C.A., Feng, X.,† Ruffieux, P.,† Fernández-Rossier, J.,† Fasel, R., *Nature* 598, 287–292. <https://doi.org/10.1038/s41586-021-03842-3>
- On-Surface Synthesis and Characterization of Super-nonazethrene**  
Turco, E.,\* Mishra, S.,\*† Melidonie, J.,\* Eimre, K., Obermann, S., Pignedoli, C.A., Fasel, R., Feng, X.,† Ruffieux, P.,† *J. Phys. Chem. Lett.* 12, 8314–8319. <https://doi.org/10.1021/acs.jpcllett.1c02381>
- Common workflows for computing material properties using different quantum engines**  
Huber, S.P.,† Bosoni, E., Bercx, M., Bröder, J., Degomme, A., Dikan, V., Eimre, K., Flage-Larsen, E., Garcia, A., Genovese, L., Gresch, D., Johnston, C., Petretto, G., Poncé, S., Rignanese, G.-M., Sewell, C.J., Smit, B., Tseplyaev, V., Uhrin, M., Wortmann, D., Yakutovich, A.V., Zadoks, A., Zarabadi-Poor, P., Zhu, B., Marzari, N., Pizzi, G.,† *npj Comput Mater* 7, 1–12. <https://doi.org/10.1038/s41524-021-00594-6>
- Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection**  
Buchs, G., Marganska, M., González, J.W., Eimre, K., Pignedoli, C.A., Passerone, D., Ayuela, A., Gröning, O., Bercieux, D.,† *Applied Physics Reviews* 8, 021406. <https://doi.org/10.1063/5.0018944>
- Large magnetic exchange coupling in rhombus-shaped nanographenes with zigzag periphery**  
Mishra, S.,\* Yao, X.,\* Chen, Q.,\* Eimre, K., Gröning, O., Ortiz, R., Di Giovannantonio, M., Sancho-García, J.C., Fernández-Rossier, J., Pignedoli, C.A., Müllen, K., Ruffieux, P., Narita, A.,† Fasel, R.,† *Nat. Chem.* 13, 581–586. <https://doi.org/10.1038/s41557-021-00678-2>
- Synthesis and characterization of [7]triangulene**  
Mishra, S.,\* Xu, K.,\* Eimre, K., Komber, H., Ma, J., Pignedoli, C.A., Fasel, R.,† Feng, X.,† Ruffieux, P.,† *Nanoscale* 13, 1624–1628. <https://doi.org/10.1039/D0NR08181G>
- On-surface synthesis of singly and doubly porphyrin-capped graphene nanoribbon segments**  
Mateo, L.M.,\* Sun, Q.,\* Eimre, K., Pignedoli, C.A., Torres,† T., Fasel, R.,† Bottari, G.,† *Chem. Sci.* 12, 247–252. <https://doi.org/10.1039/D0SC04316H>
- AiiDALab – an ecosystem for developing, executing, and sharing scientific workflows**  
Yakutovich, A.V.,\*† Eimre, K.,\* Schütt, O.,\* Talirz, L., Adorf, C.S., Andersen, C.W., Ditler, E., Du, D., Passerone, D., Smit, B., Marzari, N., Pizzi, G.,† Pignedoli, C.A.,† *Computational Materials Science* 188, 110165. <https://doi.org/10.1016/j.commatsci.2020.110165>
- 2020 **On-Surface Synthesis of Cumulene-Containing Polymers via Two-Step Dehalogenative Homocoupling of Dibromomethylene-Functionalized Tribenzoazulene**  
Urgel, J.I.,† Giovannantonio, M.D., Eimre, K., Lohr, T.G., Liu, J., Mishra, S., Sun, Q., Kinikar, A., Widmer, R., Stolz, S., Bommert, M., Berger, R., Ruffieux, P., Pignedoli, C.A., Müllen, K., Feng, X.,† Fasel, R.,† *Angewandte Chemie* 132, 13383–13389. <https://doi.org/10.1002/ange.202001939>
- Coupled Spin States in Armchair Graphene Nanoribbons with Asymmetric Zigzag Edge Extensions**  
Sun, Q.,\* Yao, X.,\* Gröning, O., Eimre, K., Pignedoli, C.A., Müllen, K., Narita, A.,† Fasel, R., Ruffieux, P.,† *Nano Lett.* 20, 6429–6436. <https://doi.org/10.1021/acs.nanolett.0c02077>
- Collective All-Carbon Magnetism in Triangulene Dimers**  
Mishra, S.,\* Beyer, D.,\* Eimre, K., Ortiz, R., Fernández-Rossier, J., Berger, R., Gröning, O., Pignedoli, C.A., Fasel, R., Feng, X.,† Ruffieux, P.,† *Angewandte Chemie International Edition* 59, 12041–12047. <https://doi.org/10.1002/anie.202002687>

**On-Surface Synthesis of Non-Benzenoid Nanographenes by Oxidative Ring-Closure and Ring-Rearrangement Reactions**

Lohr, T.G.,\* Urgel, J.I.,\*† Eimre, K.,\* Liu, J.,† Di Giovannantonio, M., Mishra, S., Berger, R., Ruffieux, P., Pignedoli, C.A., Fasel, R.,† Feng, X.,† *J. Am. Chem. Soc.* 142, 13565–13572. <https://doi.org/10.1021/jacs.0c05668>

**Reaction Pathway toward Seven-Atom-Wide Armchair Graphene Nanoribbon Formation and Identification of Intermediate Species on Au(111)**

Thussing, S., Flade, S., Eimre, K., Pignedoli, C.A., Fasel, R., Jakob, P.,† *J. Phys. Chem. C* 124, 16009–16018. <https://doi.org/10.1021/acs.jpcc.0c04596>

**Large-Cavity Coronoids with Different Inner and Outer Edge Structures**

Di Giovannantonio, M.,\*† Yao, X.,\* Eimre, K.,\* Urgel, J.I., Ruffieux, P., Pignedoli, C.A.,† Müllen, K.,† Fasel, R., Narita, A.,† *J. Am. Chem. Soc.* 142, 12046–12050. <https://doi.org/10.1021/jacs.0c05268>

**Atomic-resolution differential phase contrast STEM on ferroelectric materials: A mean-field approach**

Campanini, M.,† Eimre, K., Bon, M., Pignedoli, C.A., Rossell, M.D., Erni, R., *Phys. Rev. B* 101, 184116. <https://doi.org/10.1103/PhysRevB.101.184116>

**On-Surface Synthesis of Unsaturated Carbon Nanostructures with Regularly Fused Pentagon–Heptagon Pairs**

Hou, I.C.-Y.,\* Sun, Q.,\* Eimre, K., Di Giovannantonio, M., Urgel, J.I., Ruffieux, P., Narita, A.,† Fasel, R.,† Müllen, K.,† *J. Am. Chem. Soc.* 142, 10291–10296. <https://doi.org/10.1021/jacs.0c03635>

**Massive Dirac Fermion Behavior in a Low Bandgap Graphene Nanoribbon Near a Topological Phase Boundary**

Sun, Q., Gröning, O., Overbeck, J., Braun, O., Perrin, M.L., Barin, G.B., Abbassi, M.E., Eimre, K., Ditler, E., Daniels, C., Meunier, V., Pignedoli, C.A., Calame, M., Fasel, R., Ruffieux, P.,† *Advanced Materials* 32, 1906054. <https://doi.org/10.1002/adma.201906054>

**On-Surface Synthesis and Characterization of Triply Fused Porphyrin–Graphene Nanoribbon Hybrids**

Mateo, L.M.,\* Sun, Q.,\* Liu, S.-X., Bergkamp, J.J., Eimre, K., Pignedoli, C.A., Ruffieux, P., Decurtins, S.,† Bottari, G.,† Fasel, R.,† Torres, T.,† *Angewandte Chemie International Edition* 59, 1334–1339. <https://doi.org/10.1002/anie.201913024>

**Topological frustration induces unconventional magnetism in a nanographene**

Mishra, S.,\* Beyer, D.,\* Eimre, K., Kezilebieke, S., Berger, R., Gröning, O., Pignedoli, C.A., Müllen, K., Liljeroth, P., Ruffieux, P., Feng, X.,† Fasel, R.,† *Nature Nanotechnology* 15, 22–28. <https://doi.org/10.1038/s41565-019-0577-9>

**On-surface synthesis of super-heptazethrene**

Mishra, S.,\* Melidonie, J.,\* Eimre, K., Obermann, S., Gröning, O., A. Pignedoli, C., Ruffieux, P., Feng, X.,† Fasel, R.,† *Chemical Communications* 56, 7467–7470. <https://doi.org/10.1039/D0CC02513E>

2019 **Ab initio calculation of field emission from metal surfaces with atomic-scale defects**

Toijala, H., Eimre, K., Kyritsakis, A.,† Zadin, V., Djurabekova, F., *Phys. Rev. B* 100, 165421. <https://doi.org/10.1103/PhysRevB.100.165421>

**On-Surface Synthesis of Antiaromatic and Open-Shell Indeno[2,1-b]fluorene Polymers and Their Lateral Fusion into Porous Ribbons**

Di Giovannantonio, M.,† Eimre, K., Yakutovich, A.V., Chen, Q., Mishra, S., Urgel, J.I., Pignedoli, C.A., Ruffieux, P., Müllen, K., Narita, A.,† Fasel, R.,† *J. Am. Chem. Soc.* 141, 12346–12354. <https://doi.org/10.1021/jacs.9b05335>

**Synthesis and Characterization of  $\pi$ -Extended Triangulene**

Mishra, S.,\* Beyer, D.,\* Eimre, K., Liu, J., Berger, R., Gröning, O., Pignedoli, C.A., Müllen, K., Fasel, R., Feng, X.,† Ruffieux, P.,† *J. Am. Chem. Soc.* 141, 10621–10625. <https://doi.org/10.1021/jacs.9b05319>

### On-Surface Synthesis of a Nonplanar Porous Nanographene

Xu, K.,\* Urgel, J.I.,\* Eimre, K., Di Giovannantonio, M., Keerthi, A., Komber, H., Wang, S., Narita, A., Berger, R., Ruffieux, P., Pignedoli, C.A., Liu, J., Müllen, K.,<sup>†</sup> Fasel, R.,<sup>†</sup> Feng, X.,<sup>†</sup> *J. Am. Chem. Soc.* 141, 7726–7730. <https://doi.org/10.1021/jacs.9b03554>

### On-surface synthesis of polyazulene with 2,6-connectivity

Sun, Q.,\* Cheng-Yi Hou, I.,\* Eimre, K., A. Pignedoli, C., Ruffieux, P., Narita, A.,<sup>†</sup> Fasel, R.,<sup>†</sup> *Chemical Communications* 55, 13466–13469. <https://doi.org/10.1039/C9CC07168G>

### 2018 Dynamic coupling of a finite element solver to large-scale atomistic simulations

Veske, M.,<sup>†</sup> Kyritsakis, A., Eimre, K., Zadin, V., Aabloo, A., Djurabekova, F., *Journal of Computational Physics* 367, 279–294. <https://doi.org/10.1016/j.jcp.2018.04.031>

### Bottom-Up Synthesis of Heteroatom-Doped Chiral Graphene Nanoribbons

Wang, X.-Y.,\* Urgel, J.I.,\* Barin, G.B., Eimre, K., Di Giovannantonio, M., Milani, A., Tommasini, M., Pignedoli, C.A., Ruffieux, P., Feng, X., Fasel, R.,<sup>†</sup> Müllen, K.,<sup>†</sup> Narita, A.,<sup>†</sup> *J. Am. Chem. Soc.* 140, 9104–9107. <https://doi.org/10.1021/jacs.8b06210>

### Thermal runaway of metal nano-tips during intense electron emission

Kyritsakis, A.,<sup>†</sup> Veske, M., Eimre, K., Zadin, V., Djurabekova, F., *J. Phys. D: Appl. Phys.* 51, 225203. <https://doi.org/10.1088/1361-6463/aac03b>

### 2016 Updated baseline for a staged Compact Linear Collider

Boland, M. J. et al., CERN-2016-004. <http://dx.doi.org/10.5170/CERN-2016-004>

### Atomistic modeling of metal surfaces under high electric fields: Direct coupling of electric fields to the atomistic simulations

Veske, M.,<sup>†</sup> Kyritsakis, A., Djurabekova, F., Aare, R., Eimre, K., Zadin, V., *29th International Vacuum Nanoelectronics Conference (IVNC)*. <https://doi.org/10.1109/IVNC.2016.7551501>

### 2015 Application of the general thermal field model to simulate the behaviour of nanoscale Cu field emitters

Eimre, K., Parviainen, S.,<sup>†</sup> Aabloo, A., Djurabekova, F., Zadin, V., *Journal of Applied Physics* 118, 033303. <https://doi.org/10.1063/1.4926490>

## PRESENTATIONS

2024 **Invited talk** "Generating and publishing datasets using AiiDA and Materials Cloud" CECAM flagship workshop: Machine Learning Interatomic Potentials and Accessible Databases, Université Grenoble Alpes, France. <https://www.cecama.org/workshop-details/machine-learning-interatomic-potentials-and-accessible-databases-1313>

**Invited seminar** "High-throughput, reproducible and open computational materials research" Physicum seminar, University of Tartu, Estonia. <https://utv.ee/naita?id=35411>

2022 **Tutorial talk** "Materials Cloud and AiiDALab" Advanced Quantum ESPRESSO tutorial, online. <https://sites.google.com/view/hubbard-koopmans/>, <https://www.youtube.com/watch?v=ZgNTQ7btYds>

**Contributed talk** "Computational perspective of engineering novel graphene-based nanostructures" On-Surface Synthesis 2022, Sant Feliu De Guixols, Spain. <http://oss22.dipc.org/>

**Contributed talk** "Magnetism in graphene-based nanostructures" Psi-k 2022, EPFL, Switzerland. <https://www.psi2022.net/>

2020 **Invited talk** "AiiDALab - an Ecosystem for Developing, Executing and Sharing Scientific Workflows" Empa Access Abstraction to HPC Resources, online. <https://indico.psi.ch/event/8220/>

**Seminar talk** "On-surface synthesis of non-benzenoid nanographenes by oxidative ring-closure and ring-rearrangement reactions" MARVEL Junior Seminar, online. <https://www.nccr-marvel.ch/events/marvel-junior-seminar-aug2020>

2019 **Poster** "Examples of on-surface chemistry within AiiDALab" MARVEL Review and Retreat 2019, Lausanne. <https://www.sites.google.com/view/marvel-rr2019>

**Contributed talk** "On-surface synthesis and characterization of N-doped undecacene: a combined experimental and theoretical study" SPS2019 - Joint annual meeting of Swiss and Austrian Physical Society 2019, University of Zurich. <https://www.sps.ch/en/events/joint-annual-meeting-2019>

**Poster** "On-surface synthesis and characterization of anti-aromatic open-shell polymers: a combined experimental and computational study" Summer School on Advanced Electronic Structure Methods in Condensed Matter Physics, Lausanne. <https://sites.google.com/view/eth-electronic-structure-2019/home>

**Contributed talk** "On-surface synthesis and characterization of antiaromatic and open-shell indeno[2,1-b]fluorene polymers" Simons Collaboration Many Electron Summer School, Stony Brook University. <https://www.simonsfoundation.org/event/2019-many-electron-collaboration-summer-school/>

**Contributed talk** "On-surface synthesis and characterization of antiaromatic and open-shell indeno[2,1-b]fluorene polymers" Sixth C4 Workshop, Zurich. <https://www.c4.ethz.ch/education/seminars.html>

2018 **Poster & demo** "Jupyter and AiiDA based ecosystem for high-throughput characterization of graphene nanoribbons and molecules on surfaces" CCMX – NCCR MARVEL Materials Science Day, Bern. <https://www.epfl.ch/research/domains/ccmx/past-courses-and-events/ccmx-nccr-marvel-materials-science-day-2018/>

**Poster & demo** "Jupyter and AiiDA based ecosystem for high-throughput characterization of graphene nanoribbons and molecules on surfaces" COMDI2018 - International Workshop on Computational Design and Discovery of Novel Materials, Lausanne. <https://sites.google.com/view/comdi2018>

**Poster** "Computational characterization of one-dimensional carbon nanostructures: examples together with experiments and high-throughput automation based on AiiDA" Paris International School on Advanced Computational Materials Science, Paris. [https://pisacms.sciencesconf.org/data/pages/livret\\_PISACMS\\_2018.pdf](https://pisacms.sciencesconf.org/data/pages/livret_PISACMS_2018.pdf)

**Contributed talk** "On-surface synthesis and characterization of indenofluorene-based polymers: a combined experimental and computational study" 13th mol CH surfaces meeting, Bern. <https://www.empa.ch/web/molch/molchmeeting>

**Contributed talk** "Doubled quasi-bound states in metallic zigzag carbon nanotubes: an ab initio perspective" DPG Spring Meeting of the Condensed Matter Section, Berlin. <https://www.dpg-verhandlungen.de/year/2018/conference/berlin/part/tt/session/33/contribution/2>

2015 **Contributed talk** "Implementing the general thermal-field emission equation to the high electric field nanopenetration model" MeVArc 2015, Saariselkä. <https://indico.cern.ch/event/354854/contributions/834823/>