# KRISTJAN EIMRE

CURRICULUM VITAE

## PERSONAL DATA


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|---|---|
| **e-mail** | kristjaneimre@gmail.com |
| **website** | https://kristjaneimre.eu |
| **GitHub** | https://github.com/eimrek |
| **languages** | English (C1), Estonian (native) |


## EDUCATION

2017 – NOW **Ph.D. in Chemistry**, Swiss Federal Laboratories for Materials Science and Technology (Empa) and University of Zurich

2015 – 2017 **M.Sc. in Physics**, University of Tartu, GPA: 5.0/5.0, *cum laude*
thesis: "Multiscale electrical and thermal simulations of metal surface defects in high electric field" https://dspace.ut.ee/handle/10062/56621

2011 – 2015 **B.Sc. in Physics**, minor in Comp. Sci., University of Tartu, GPA: 4.85/5.00, *cum laude*
thesis: "Implementing the general thermal-field emission equation to the high electric field nanoprotrusion model" https://dspace.ut.ee/handle/10062/47429

2008 – 2011 Hugo Treffner Gymnasium, Tartu

## EMPLOYMENT

2017 – NOW **Junior Researcher** at Swiss Federal Laboratories for Materials Science and Technology (Empa), nanotech@surface laboratory, https://www.empa.ch/web/s205
Studying carbon nanomaterials with density functional theory (DFT) and beyond-DFT methods; building automation tools for materials' computation.

2014 – 2017 **Research Assistant** at University of Tartu, Intelligent Materials and Systems Lab
Studying metal surface defects with finite element, density functional theory and quantum transport methods.

2016 SUMMER **Intern** at Aalto University, Multiscale Statistical and Quantum Physics group
Implementing and improving phase field crystal models.

2015 SUMMER **Intern** at the CMS collaboration, CERN
Engineering project to build a hardware and software solution for sensor calibration.

## NOTABLE PROJECTS

2017 – NOW **Computational characterization of carbon nanomaterials**
PYTHON, CP2K, QUANTUM ESPRESSO, GAUSSIAN, ORCA
Using density functional theory, GW and multiconfigurational methods to characterize novel organic systems and phenomena pertaining on-surface synthesis. Strong collaboration with experimental colleagues has enabled me to co-author over 20 scientific publications in various high-impact journals.
https://doi.org/10.1021/jacs.0c05268
https://doi.org/10.1021/jacs.0c05668
https://www.nature.com/articles/s41565-019-0577-9

2017 – NOW
PYTHON

**Automation of computational materials science: AiiDA & AiiDAlab**
Leveraging the AiiDA infrastructure to develop high-throughput automation workflows for atomistic simulations of materials. Additionally, I am a main contributor to AiiDAlab, a web platform hosting an ecosystem of user-friendly apps for complex workflows.
https://doi.org/10.1016/j.commatsci.2020.110165
https://www.materialscloud.org/work/aiidalab

2014 – 2017
PYTHON, C++, VASP, COMSOL

**Electrical and thermal simulations of surface defects in high electric field**
Used finite element analysis, density functional theory and quantum-transport simulations to study the physical mechanisms contributing to the detrimental vacuum breakdown phenomena. Co-authored a total of 6 scientific journal and conference papers.
https://github.com/eimrek/dealii-field-currents-heating

2016
C++, PYTHON, MPI

**Improved mechanical equilibration algorithms for phase field crystal modelling**
Developed a high-performance parallel code to perform phase field crystal modelling and benchmarked various optimization algorithms for equilibration.
https://kristjaneimre.eu/c/pfc.pdf
https://github.com/eimrek/phase-field-crystal-mpi

2015
HARDWARE

**Laboratory setup for temperature and humidity measurements**
CERN internship project, where I built a hardware and software solution to conveniently calibrate dozens of temperature and humidity sensors together.
https://cds.cern.ch/record/2046232

2014
C++, ML

**Word recognition using neural networks**
Group project in course "Signal processing I". I was responsible for programming the neural networks and the genetic algorithm to train them.
https://kristjaneimre.eu/c/word_recog.pdf

2012
PYTHON, HARDWARE

**Robotex soccer competition**
Soccer tournament for autonomous robots. The competition entails designing, building and programming the robot. I was a member of the team "Kübaratrikk", we achieved 4th place out of 33 teams.

## PUBLICATIONS

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

2021 Mishra, S.,* Xu, K.,* Eimre, K., Komber, H., Ma, J., Pignedoli, C.A., Fasel, R.,† Feng, X.,† Ruffieux, P.,† **Synthesis and characterization of [7]triangulene**. Nanoscale 13, 1624–1628. https://doi.org/10.1039/D0NR08181G

Mateo, L.M.,* Sun, Q.,* Eimre, K., Pignedoli, C.A., Torres,† T., Fasel, R.,† Bottari, G.,† **On-surface synthesis of singly and doubly porphyrin-capped graphene nanoribbon segments**. Chem. Sci. 12, 247–252. https://doi.org/10.1039/D0SC04316H

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.,† **AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows**. Computational Materials Science 188, 110165. https://doi.org/10.1016/j.commatsci.2020.110165

2020 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.,† **On-Surface Synthesis of Cumulene-Containing Polymers via Two-Step Dehalogenative Homocoupling of Dibromomethylene-Functionalized Tribenzoazulene**. Angewandte Chemie 132, 13383–13389. https://doi.org/10.1002/ange.202001939

Sun, Q.,* Yao, X.,* Gröning, O., Eimre, K., Pignedoli, C.A., Müllen, K., Narita, A.,† Fasel, R., Ruffieux, P.,† **Coupled Spin States in Armchair Graphene Nanoribbons with Asymmetric Zigzag Edge Extensions**. Nano Lett. 20, 6429–6436. https://doi.org/10.1021/acs.nanolett.0c02077

Mishra, S.,* Beyer, D.,* Eimre, K., Ortiz, R., Fernández-Rossier, J., Berger, R., Gröning, O., Pignedoli, C.A., Fasel, R., Feng, X.,† Ruffieux, P.,† **Collective All-Carbon Magnetism in Triangulene Dimers**. Angewandte Chemie International Edition 59, 12041–12047. https://doi.org/10.1002/anie.202002687

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.,† **On-Surface Synthesis of Non-Benzenoid Nanographenes by Oxidative Ring-Closure and Ring-Rearrangement Reactions**. J. Am. Chem. Soc. 142, 13565–13572. https://doi.org/10.1021/jacs.0c05668

Thussing, S., Flade, S., Eimre, K., Pignedoli, C.A., Fasel, R., Jakob, P.,† **Reaction Pathway toward Seven-Atom-Wide Armchair Graphene Nanoribbon Formation and Identification of Intermediate Species on Au(111)**. J. Phys. Chem. C 124, 16009–16018. https://doi.org/10.1021/acs.jpcc.0c04596

Di Giovannantonio, M.,*† Yao, X.,* Eimre, K.,* Urgel, J.I., Ruffieux, P., Pignedoli, C.A.,† Müllen, K.,† Fasel, R., Narita, A.,† **Large-Cavity Coronoids with Different Inner and Outer Edge Structures**. J. Am. Chem. Soc. 142, 12046–12050. https://doi.org/10.1021/jacs.0c05268

Campanini, M.,† Eimre, K., Bon, M., Pignedoli, C.A., Rossell, M.D., Erni, R., **Atomic-resolution differential phase contrast STEM on ferroelectric materials: A mean-field approach**. Phys. Rev. B 101, 184116. https://doi.org/10.1103/PhysRevB.101.184116

Hou, I.C.-Y.,* Sun, Q.,* Eimre, K., Di Giovannantonio, M., Urgel, J.I., Ruffieux, P., Narita, A.,† Fasel, R.,† Müllen, K.,† **On-Surface Synthesis of Unsaturated Carbon Nanostructures with Regularly Fused Pentagon–Heptagon Pairs**. J. Am. Chem. Soc. 142, 10291–10296. https://doi.org/10.1021/jacs.0c03635

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.,† **Massive Dirac Fermion Behavior in a Low Bandgap Graphene Nanoribbon Near a Topological Phase Boundary**. Advanced Materials 32, 1906054. https://doi.org/10.1002/adma.201906054

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.,† **On-Surface Synthesis and Characterization of Triply Fused Porphyrin–Graphene Nanoribbon Hybrids**. Angewandte Chemie International Edition 59, 1334–1339. https://doi.org/10.1002/anie.201913024

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.,† **Topological frustration induces unconventional magnetism in a nanographene**. Nature Nanotechnology 15, 22–28. https://doi.org/10.1038/s41565-019-0577-9

Mishra, S.,* Melidonie, J.,* Eimre, K., Obermann, S., Gröning, O., A. Pignedoli, C., Ruffieux, P., Feng, X.,† Fasel, R.,† **On-surface synthesis of super-heptazethrene**. Chemical Communications 56, 7467–7470. https://doi.org/10.1039/D0CC02513E

2019 Toijala, H., Eimre, K., Kyritsakis, A.,† Zadin, V., Djurabekova, F., **Ab initio calculation of field emission from metal surfaces with atomic-scale defects**. Phys. Rev. B 100, 165421. https://doi.org/10.1103/PhysRevB.100.165421

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.,† **On-Surface Synthesis of Antiaromatic and Open-Shell Indeno[2,1-b]fluorene Polymers and Their Lateral Fusion into Porous Ribbons**. J. Am. Chem. Soc. 141, 12346–12354. https://doi.org/10.1021/jacs.9b05335

Mishra, S.,* Beyer, D.,* Eimre, K., Liu, J., Berger, R., Gröning, O., Pignedoli, C.A., Müllen, K., Fasel, R., Feng, X.,† Ruffieux, P.,† **Synthesis and Characterization of $\pi$-Extended Triangulene**. J. Am. Chem. Soc. 141, 10621–10625. https://doi.org/10.1021/jacs.9b05319

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.,† Fasel, R.,† Feng, X.,† **On-Surface Synthesis of a Nonplanar Porous Nanographene**. J. Am. Chem. Soc. 141, 7726–7730. https://doi.org/10.1021/jacs.9b03554

Sun, Q.,* Cheng-Yi Hou, I.,* Eimre, K., A. Pignedoli, C., Ruffieux, P., Narita, A.,† Fasel, R.,† **On-surface synthesis of polyazulene with 2,6-connectivity**. Chemical Communications 55, 13466–13469. https://doi.org/10.1039/C9CC07168G

2018 Veske, M.,† Kyritsakis, A., Eimre, K., Zadin, V., Aabloo, A., Djurabekova, F., **Dynamic coupling of a finite element solver to large-scale atomistic simulations**. Journal of Computational Physics 367, 279–294. https://doi.org/10.1016/j.jcp.2018.04.031

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.,† Müllen, K.,† Narita, A.,† **Bottom-Up Synthesis of Heteroatom-Doped Chiral Graphene Nanoribbons**. J. Am. Chem. Soc. 140, 9104–9107. https://doi.org/10.1021/jacs.8b06210

Kyritsakis, A.,† Veske, M., Eimre, K., Zadin, V., Djurabekova, F., **Thermal runaway of metal nano-tips during intense electron emission**. J. Phys. D: Appl. Phys. 51, 225203. https://doi.org/10.1088/1361-6463/aac03b

2016 M. J. Boland et al. [including Eimre, K.], **Updated baseline for a staged Compact Linear Collider**. CERN-2016-004. http://dx.doi.org/10.5170/CERN-2016-004

Veske, M.,† Kyritsakis, A., Djurabekova, F., Aare, R., Eimre, K., Zadin, V., **Atomistic modeling of metal surfaces under high electric fields: Direct coupling of electric fields to the atomistic simulations**, 29th International Vacuum Nanoelectronics Conference (IVNC). https://doi.org/10.1109/IVNC.2016.7551501

2015 Eimre, K., Parviainen, S.,† Aabloo, A., Djurabekova, F., Zadin, V., **Application of the general thermal field model to simulate the behaviour of nanoscale Cu field emitters**. Journal of Applied Physics 118, 033303. https://doi.org/10.1063/1.4926490

## TALKS & POSTERS

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

**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 nanoprotrusion model" MeVArc 2015, Saariselkä. https://indico.cern.ch/event/354854/contributions/834823/

## TEACHING

2018/19 Statistical Mechanics and Molecular Simulations (University of Zurich; CHE327)

Condensed Matter Electronic Structure Theory (University of Zurich; CHE437)

2017/18 Molecular and Materials Modelling (ETH Zurich; 327-5102-00L)

2015/16 Computational Physics I (University of Tartu; LOTI.05.030)

## THESIS SUPERVISION

2019/20 Mean-field Hubbard model implementation and application to carbon-based nanostructures

Robin Worreby, B.Sc. in Computational Science at ETH Zurich

*Last updated March 31, 2021*