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#### Added personal information:

*Nationality:* Czech Republic  
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#### Degrees

11/2017 Ph.D., Physics of Surfaces and Interfaces, Charles University, Czech Republic, email: [stud@dekanat.mff.cuni.cz](mailto:stud@dekanat.mff.cuni.cz), phone: +420 95155 1254, Thesis title: *DFTsimulations of interactions between organic molecules and oriented surfaces*  
05/2013 Master, Biophysics and Chemical Physics – Theory of Molecular Systems, Charles University, Czech Republic  
09/2011 Bachelor, General Physics, Charles University, Czech Republic

#### Current employment

Since 03/2022 Post-doctoral researcher/Research Fellow (since 02/2023), Alcon project, Department of Applied Physics, Aalto University, Finland

#### Previous work experience

01/2020 – 03/2022 Marie Skłodowska-Curie Fellow, 845060 project – QMKPFM, Department of Applied Physics, Aalto University, Finland  
01/2018 – 12/2019 Post-doctoral researcher, Academy of Finland's COMP center of excellence, Department of Applied Physics, Aalto University, Finland  
10/2010 – 12/2017 Research assistant, part-time, NanosurfLab, Institute of Physics of the AS CR, Czech Republic (Erasmus Break 09/2013 – 06/2014)

#### Research funding and grants

01/2020 – 03/2022 Marie Skłodowska-Curie Action, 845060 project, Individual Fellowship, Horizon 2020, 202 681.96 €, Principal investigator, 8 papers published.  
03/2012 – 03/2015 Charles University, Prague, Czech Republic, Student Grant (GaUK #667012)

#### Research output

- 23 peer-reviewed publications (+1 correction) with 1213/881 citations as of Google Scholar/Web of Science 12/08/2024 and *h*-index of 15/14; three examples:
  - i. Q. Fan, L. Yan, M.W. Tripp, **O. Krejci**, S. Dimosthenous, S. R. Kachel, M. Chen, A. S. Foster, U. Koert, P. Liljeroth, Peter; M. J. Gottfried, *Biphenylene network: A nonbenzenoid carbon allotrope*, **Science** **372**, 852-856 (2021)
  - ii. **O. Krejčí**, P. Hapala, M. Ondráček and P. Jelínek. *Principles and simulations of high-resolution STM imaging with a flexible tip apex*, **Phys. Rev. B** **95**, 045407 (2017), Open Access URL
  - iii. N. Oinonen, A. V. Yakutovich, A. Gallardo, M. Ondráček, P. Hapala, **O. Krejčí**, **Comp. Phys. Commun.** 109341 (2024)
- Software developer:
  - a. PPSTM simulation software, main developer.
  - b. KPFM\_sim simulation software, main developer, main outcome of my MSC Fellowship.
  - c. ppafm simulation software, developer and maintainer.

#### Research supervision and leadership experience

08/2022 – on-going Supervisor of Ph.D. student, Prajwal Pisal, Aalto University, Finland  
10/2022 – on-going Supervisor of Ph.D. student, Nitik Bhatia, Aalto University, Finland and under the auspices of the EUSpecLab ITN.  
06/2023 – 09/2023 Bachelor student supervisor, Barnik Brata, Aalto University, Finland  
06/2021 – 09/2021 Bachelor student supervisor, Nico Toikka, Aalto and Helsinki University, Finland  
07/2020 – 08/2020 Summer student supervisor, Konrad Kusiak, Aalto University, Finland  
06/2018 – 03/2022 Advisor to Bachelor, Master, Ph.D. students and occasionally post-docs, SIN group, Aalto University, Finland  
03/2012 – 03/2015 Leader of a 3 persons team within the GaUK #667012 student grant, Charles University, Czech Republic.

#### Teaching merits and pedagogy training:

03/2024 – on-going co-developer of a new course – Advanced Computational Methods in Physics, Aalto University, Finland  
09/2019 – 12/2023 Teacher and course co-developer of Density-Functional Theory course, workload 64h/semester, Aalto University, Finland  
01/2020 – 06/2021 Teacher/Tutor for students creating artificial research enhancing encyclopedia, EIT-AMIS Inno-project, workload 41h/semester, Aalto University, Finland

04/2024 Course: AI Peda Intro, Aalto University, Finland  
12/2023 Course: Doctoral supervision, Aalto University, Finland  
03/2022 Course: Teaching assistant as a learning instructor, Aalto University, Finland

#### Other key academic merits

- Invited talks: NANO KOREA 2018, THIS 2018 Workshop, Korea and two university seminars – 2021 Charles University, Czech Republic and 2022 Ulm University, Germany.
- Programming skills: Python, C++, Fortran, Mathematica, CUDA
- Referee for scientific journals: 31 reviews
- Chairman at conferences: plenary chairman – once – and session chairman – twice.

#### Scientific and social impact

02/2023 Member of committee choosing the best master thesis in Finland as a part of Finnish Physical Society Board  
12/2023 School of Science Award for the work on Making Waves, Aalto University  
04/2023 – on-going Elected board member and communication manager of the Finnish Physical Society Board  
06/2022 – on-going Member of the FinDiP committee (chair 11/2023 – 05/2024): Organization of public talk  
09/2022 – on-going part of Aalto University Junior: Researcher talks; 2 talks + student supervision  
06/2020 – 06/2023 Co-organiser of Making Waves: a series of public talks addressing diversity and inclusiveness issues at Aalto University  
01/2020 – 03/2022 5 databases published as part of Pilot on Open Research Data in Horizon 2020

#### Other education and expertise

05/2023 Soft-skills training for supervisor, Centrum dohody, Prague, Czech Republic  
04/2023 Month exchange in John Kitchin's group – Machine Learning in Computational Catalysis, Carnegie Mellon University, USA  
12/2022 Participant: Workflow workshop/hackathon, CSC, Finland  
12/2019 Course: Machine Learning for Materials Science, Aalto University, Finland  
09/2013 – 05/2014 Erasmus, group of prof. L. G. M. Pettersson, Stockholm University, Sweden

#### Language skills

*Native:* Czech

*Fluent:* English

*Intermediate:* Finnish

*Basic:* Swedish, German, Latvian

## Research outputs

### Advancing scanning probe microscopy simulations : A decade of development in probe-particle models

Oinonen, N., Yakutovich, A. V., Gallardo, A., Ondráček, M., Hapala, P. & Krejčí, O., Dec 2024, In: Computer Physics Communications. 305, p. 1-12 12 p., 109341.

### Differences in Molecular Adsorption Emanating from the (2 × 1) Reconstruction of Calcite(104)

Heggemann, J., Ranawat, Y. S., Krejčí, O., Foster, A. S. & Rahe, P., 23 Feb 2023, In: Journal of Physical Chemistry Letters. 14, 7, p. 1983-1989 7 p.

### On-surface synthesis of disilabenzene-bridged covalent organic frameworks

Sun, K., Silveira, O. J., Ma, Y., Hasegawa, Y., Matsumoto, M., Kera, S., Krejčí, O., Foster, A. S. & Kawai, S., Jan 2023, In: Nature Chemistry. 15, 1, p. 136-142 7 p.

### Electrostatic Discovery Atomic Force Microscopy

Oinonen, N., Xu, C., Alldritt, B., Canova, F. F., Urtev, F., Cai, S., Krejčí, O., Kannala, J., Liljeroth, P., Foster, A. S. & Hapala, H., 25 Jan 2022, In: ACS Nano. 16, 1, p. 89-97 9 p.

### Integrating Bayesian Inference with Scanning Probe Experiments for Robust Identification of Surface Adsorbate Configurations

Järvi, J., Alldritt, B., Krejčí, O., Todorović, M., Liljeroth, P. & Rinke, P., 9 Aug 2021, In: Advanced Functional Materials. 31, 32, 8 p., 2010853.

### **Synthesis and Local Probe Gating of a Monolayer Metal-Organic Framework**

Yan, L., Silveira, O. J., Alldritt, B., Krejčí, O., Foster, A. S. & Liljeroth, P., 26 May 2021, In: *Advanced Functional Materials*. 31, 22, p. 2100519 7 p., 2100519.

### **Biphenylene network: A nonbenzenoid carbon allotrope**

Fan, Q., Yan, L., Trip, M. R., Krejci, O., Dimosthenous, S., Kachel, S. R., Chen, M., Foster, A., Liljeroth, P. & Gottfried, J. M., 21 May 2021, In: *Science*. 372, 6544, p. 852-856 44 p.

### **On-Surface Synthesis of a $\pi$ -Extended Diaza[8]circulene**

Nakamura, K., Li, Q. Q., Krejčí, O., Foster, A. S., Sun, K., Kawai, S. & Ito, S., 15 May 2020, In: *Journal of the American Chemical Society*. 142, 26, p. 11363–11369

### **Three-dimensional graphene nanoribbons as a framework for molecular assembly and local probe chemistry**

Kawai, S., Krejci, O., Nishiuchi, T., Sahara, K., Kodama, T., Pawlak, R., Meyer, E., Kubo, T. & Foster, A., 28 Feb 2020, In: *Science Advances*. 6, 9, 7 p., eaay8913.

### **Automated structure discovery in atomic force microscopy**

Alldritt, B., Hapala, H., Oinonen, N., Urtev, F., Krejci, O., Federici Canova, F., Kannala, J., Schulz, F., Liljeroth, P. & Foster, A., 26 Feb 2020, In: *Science Advances*. 6, 9, 10 p., eaay6913.

### **Synthesis of Regioisomeric Graphene Nanoribbon Junctions via Heteroprecursors**

Sun, K., Krejci, O., Foster, A. S., Okuda, Y., Orita, A. & Kawai, S., 18 Jul 2019, In: *Journal of Physical Chemistry C*. 123, 28, p. 17632-17638 7 p.

### **Interface dipoles of $\text{Ir}(\text{ppy})_3$ on $\text{Cu}(111)$**

Queck, F., Albrecht, F., Mutombo, P., Krejci, O., Jelínek, P., McLean, A. & Repp, J., 14 Jul 2019, In: *Nanoscale*. 11, 26, p. 12695-12703 9 p.

### **Bonding Motifs in Metal-Organic Compounds on Surfaces**

Queck, F., Krejčí, O., Scheuerer, P., Bolland, F., Otyepka, M., Jelínek, P. & Repp, J., 17 Sept 2018, In: *Journal of the American Chemical Society*. 140, p. 12884–12889 40.

### **Diacetylene Linked Anthracene Oligomers Synthesized by One-Shot Homocoupling of Trimethylsilyl on $\text{Cu}(111)$**

Kawai, S., Krejci, O., Foster, A., Pawlak, R., Xu, F., Peng, L., Orita, A. & Meyer, E., 7 Aug 2018, In: *ACS Nano*. 12, 8, p. 8791–8797

### **Elemental Identification by Combining Atomic Force Microscopy and Kelvin Probe Force Microscopy**

Schulz, F., Ritala, J., Krejčí, O., Seitsonen, A. P., Foster, A. S. & Liljeroth, P., 26 Jun 2018, In: *ACS Nano*. 12, 6, p. 5274-5283 10 p.

#### **Pre-Aalto publications:**

B. de la Torre, M. Švec, G. Foti, O. Krejčí, P. Hapala, A. Garcia-Lekue, T. Frederiksen, R. Zbořil, A. Arnau, H. Vázquez, and P. Jelínek, Submolecular Resolution by Variation of the Inelastic Electron Tunneling Spectroscopy Amplitude and its Relation to the AFM/STM Signal, *Phys. Rev. Lett.* 119, 166001 (2017)

DOI: <http://dx.doi.org/10.1103/PhysRevLett.119.166001> (Open Access)

J. LaRue, O. Krejčí, L. Yu, M. Beye, M. L. Ng, H. Öberg, H. Xin, G. Mercurio, S. Moeller, J. J. Turner, D. Nordlund, R. Coffee, M. P. Minitti, W. Wurth, L. G. M. Pettersson, H. Öström, A. Nilsson, F. Abild-Pedersen and H. Ogasawara, Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru, *J. Phys. Chem. Lett.* 8, pp 3820–3825 (2017)

DOI: <http://dx.doi.org/10.1021/acs.jpcllett.7b01549>

O. Krejčí, P. Hapala, M. Ondráček and P. Jelínek, Principles and simulations of high-resolution STM imaging with a flexible tip apex, *Phys. Rev. B* 95, 045407 (2017)

DOI: <http://dx.doi.org/10.1103/PhysRevB.95.045407>

Open Access version: <https://arxiv.org/abs/1609.09462>

O. Krejčí, P. Matvija, P. Zimmermann, P. Sobotík, I. Ošťádal and P. Kocán, Chemisorption of Acetophenone on  $\text{Si}(111)\text{-}7 \times 7$  Polar Aromatic Molecule on Electronically Complex Surface, *J. Phys. Chem. C* 120, pp 9200–9206 (2016)

DOI: <http://dx.doi.org/10.1021/acs.jpcc.6b00486>

N. Kocić, X. Liu, S. Chen, S. Decurtin, O. Krejčí, P. Jelínek, J. Repp and S.X. Liu, Control of Reactivity and Regioselectivity for On-Surface Dehydrogenative Aryl–Aryl Bond Formation, *J. Am. Chem. Soc.* 138, pp 5585–5593 (2016)

DOI: <http://dx.doi.org/10.1021/jacs.5b13461>

J. Sforzini, M. Telychko, O. Krejčí, M. Vondráček, M. Švec, F. C. Bocquet, and F. S. Tautz, Transformation of metallic boron into substitutional dopants in graphene on 6H-SiC (0001), *Phys. Rev. B* 93, 041302 (2016)

DOI: <http://dx.doi.org/10.1103/PhysRevB.93.041302> (Open Access)

P. Kocán, O. Krejčí, O. and H. Tochiara, Anomalous structural evolution and  $\sqrt{3}\times\sqrt{3}$  reconstruction of a clean Si(111) surface observed after thermal desorption of thallium, *J. Vac. Sci. Technol. A* 33, 021408 (2015)

DOI: <http://dx.doi.org/10.1116/1.4913199>