

# Curriculum Vitae

## Personal information

**Name:** Prokop Hapala  
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## Education

**Ph.D. study:** **2009-2016**, Charles University in Prague; Faculty of Mathematics and Physics; Physics of Condensed Matter and Materials Research  
**Ph.D. thesis:** Theoretical simulations of electron transport in nanostructures  
**Supervisor:** Ing. Pavel Jelínek, Ph.D.

**Master study:** **2007-2009**, Institute of Chemical Technology, Prague; Faculty of Chemical Engineering; Molecular Engineering  
**Master thesis:** Modeling of the SPM techniques for DNA analyses  
**Supervisor:** prof. RNDr. Štěpán Urban, CSc.  
**Consultant:** Ing. Pavel Jelínek, Ph.D.

**Bachelor study:** **2004-2007**, Czech Technical University; Faculty of Nuclear Sciences and Physical Engineering; Lasers and optoelectronics.  
**Bachelor thesis:** Theoretical and experimental research of pyrene derivatives  
**Supervisor:** RNDr. Martin Michl, Ph.D.  
**Consultant:** Doc. Ing. Vlastimil Fidler, CSc

## Working experience

**2019-present** Department of Condensed Matter Theory, Institute of Physics of the Czech Academy of Sciences

**2018-2019** postdoc, Department of Applied Physics, Aalto University, group of Surfaces and Interfaces at the Nanoscale (with Prof. Adam Foster)

**2017-2018** visiting researcher (5 months), Georg-August-Universität Göttingen, (with Prof. Joerg Behler)

**2016-2017** visiting researcher (4 months), University of Amsterdam, (with Dr. Kateřina Dohnalová)

**2007-2018** Department of thin films and nanostructures, Institute of Physics of the Czech Academy of Sciences, Nanosurf Lab (with Dr. Pavel Jelínek)

## Research interests and outcomes

- Theoretical description of scanning-probe microscopy**
  - explanation and simulation of sub-molecular resolution in AFM, STM and IETS using chemically modified tip (CO, Xe) ([Phys. Rev. B 2014](#), [Phys. Rev. Lett 2014](#))
  - ProbeParticleModel (<https://github.com/ProkopHapala/ProbeParticleModel/wiki>) became standard tool for theoretical support of AFM with submolecular resolution (more than 200 citations since 2014)
  - sub-molecular resolution in STM – PPSTM (<https://github.com/ondrejkrejci/PPSTM>)
  - automatic interpretation of molecular structure from AFM data using machine-learning (Science Advances [2020](#))
- Contributing to **development of fast local-orbital DFT code** ([www.fireball-dft.org](http://www.fireball-dft.org))
  - integration with non-equilibrium Green's function molecular transport code SMEAGOL
  - modules for: simulation of optical spectra, band-structure unfolding, MetaDynamics, FIRE-relaxation algorithm and more
- Non-covalent and chemical interactions of organic molecules** on inorganic crystalline surface studied using high-resolution scanning-probe microscopy
  - Weakly bonded clusters of water on ionic crystals ([Nature 2018](#); [Nat. Comm. 2018](#))
  - Electrostatic field of molecules on surface ([Nat. Comm. 2016](#), [Phys. Rev. Lett. 2016](#))
  - Molecules and reactions promising for molecular electronics ([J. Phys. Chem. C 2016](#)), photonics ([ACS Nano 2017](#)) and spintronics (2xNat. Comm. 2018: [July](#), [August](#))

## Awards

**2016** - Otto Wichterle Award (Czech Academy of Sciences)

**2021** – Czech “Neuron” Award for promising young research in Chemistry (<https://www.nfneuron.cz/person/prokop-hapala>)

## Publication activity

- **36** impacted publications (**4x first author, 1x Nature**, 1x Science Advances, 6x Nature Communications, 6x ACS Nano, 1x Chemistry of Materials, 6x Phys. Rev. Lett)
- **1915 citations, h-index 21** according to Scopus, February 2023
- **2521 citations, h-index 24** according to Google Scholar, February 2023
- referee for Physical Review Letters, Physical Review B, Physical Review Materials, Journal of Physical Chemistry

## Mentoring Students

**2014-2016** – Mentoring 2 PhD students (V. Zobač, O. Krejčí) under supervision of P. Jelínek

**2018-2019** – Mentoring Msc. student Niko Oinonen under supervision of Adam Foster

**2022-** – Supervising PhD student Mithun Manikandan

## Grants

**2019-2021** – PPLZ program of AVČR, “*Connecting reactive force fields and electronic structure methods*”

**2022-(2026)** – GAČR Junior Star grant “*Computer Aided Design of Templated Assembling, Replication and Synthesis on Ionic Substrates*”