Jiří Klimeš

BORN 21. 3. 1983 in Broumov, Czech Republic

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Professional Experience

January 2015-

Charles University, Faculty of Mathematics and Physics, Prague, CZ

Researcher (part-time during the work on the MSC grant)

April 2015–March 2017

J. Heyrovský Institute of Physical Chemistry, Prague, CZ

Marie Skłodowska Curie Fellow

June 2014–December 2014

J. Heyrovský Institute of Physical Chemistry, Prague, CZ

Visiting Researcher, continuing collaboration with Georg Kresse

Partly parental leave

January 2012-May 2014

University of Vienna, Faculty of Physics, Vienna, Austria

Postdoctoral Researcher with Georg Kresse

January 2011–December 2011

University College London, Department of Chemistry, London, UK

PhD+ Postdoctoral Fellow with Angelos Michaelides

April 2003–June 2005

Institute of Atmospheric Physics, Czech Academy of Sciences, Prague, CZ

Junior Researcher

EDUCATION

September 2007–May 2011

University College London, Department of Chemistry, London, UK

Study programme: Chemistry, PhD

Thesis: Towards an accurate theoretical description of surface processes

Supervisor: Angelos Michaelides

October 2002-June 2007

Charles University, Faculty of Mathematics and Physics, Prague, CZ

Study programme: Physics, Chemical Physics (5 year Masters)

Summa Cum Laude

Thesis: Non-elastic electron transport in molecular junctions

Supervisor: Martin Čížek

Honors and Awards 2013: Second poster prize at The VIIIth Congress of the International Society of Theoretical

Chemical Physics (ISTCP-VIII)

2012: Second place in JČMF Martin Odehnal's competition for young physicists organised

by the Czech Union of Mathematicians and Physicists

2010: Publication Prize of the UCL Chemistry Department for the best publication by a PhD student

2009: Thomas Young Centre Junior Research Fellowship

2003–2007: Scholarship for excellent study results

Grants

2024–2027: Inter-COST grant of Ministry of Education

Calculations of reference binding energies of polymorphs of molecular crystals. Total budget: 210 000 EUR.

2018–2022: ERC Starting Grant

APES: Accuracy and Precision for Molecular Solids. Total budget: 924 000 EUR.

2017–2019: Primus

Competitive start-up grant by the Charles University. Total budget: 170 000 EUR. 2015 -

15 accepted proposals for CPU time on the national HPC resources at IT4I. Total allocation over 25 mil. CPU hours.

2016–2018: Standard grant of the Czech grant agency

Declined due to the work on the MSC Fellowship. Total budget: 160 000 EUR.

2015–2017: Junior grant of the Czech grant agency

Declined due to non-transferability between institutions. Total budget: 205 000 EUR.

2011: PhD+ Postdoctoral Fellowship

A competitive grant awarded to continue and extend the work performed during PhD. Total budget ~ 30.000 GBP.

PUBLICATIONS

47 published articles in peer-reviewed journals, over 10000 citations without self-citations. $Researcher ID: \ D-8926-2011, \ ORCID: \ 0000-0003-4969-1343.$

Conference

5 invited and 16 contributed talks at international conferences.

Presentations

STUDENT

2023–2024: A. Mendl, BSc student

Supervision 2022–2023: J. Kovačovský, BSc student

2018–2024: Pham N. K., PhD student on the ERC project

2017-: K. Prokofiev, PhD student on the Primus project

2016–2019: J. Hofierka, student project, BSc thesis, MS. thesis

2010–2011: G. Graziano, PhD student, supervisor A. Michaelides

2009–2010: C. Ignatius, MSc. student, supervisor A. Michaelides

MEMBERSHIP

Institute of Physics, Royal Society of Chemistry, American Physical Society, American Chemical Society

Referee for

Science, Physical Review Letters, Physical Review B, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of Chemical Theory and Computation, Journal of Physics: Condensed Matter, Physica Status Solidi, Carbon, Computational Materials Science, Surface Science, Journal of Organometallic Chemistry

Grant Referee National Science Foundation, Austrian Science Fund

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