Jiří Klimeš

Born	21. 3. 1983 in Broumov, Czech Republic
Marital Status	Married, 1 child
Professional Experience	1. 6. 2014– **J. Heyrovský Institute of Physical Chemistry ASCR**, Prague, Czech Rep. *Visiting Researcher* Development of Green's function based methods for description of materials. *Part-time parental leave.* 16. 1. 2012–31. 5. 2014 **University of Vienna**, Faculty of Physics, Vienna, Austria *Postdoctoral Researcher* with Georg Kresse Application of many-body perturbation theory to study electronic properties of materials. Implementation and development of algorithms for calculation of correlation energies. 1. 1. 2011–31. 12. 2011 **University College London**, Department of Chemistry, London, UK *PhD+ Postdoctoral Fellow* with Angelos Michaelides Application of dispersion corrected density functional theory to surfaces and interfaces. Development of methods for description of weak interactions. 1. 4. 2003–30. 6. 2005 **Institute of Atmospheric Physics**, Department of Ionospheric Physics, Czech Academy of Sciences, Prague, CZ *Junior Researcher* Numerical calculations.
Education	September 2007–December 2010 **University College London**, Department of Chemistry, London, UK Study programme: Chemistry, PhD Date of award: 28. 5. 2011 Thesis: Towards an accurate theoretical description of surface processes Supervisor: Angelos Michaelides October 2002–June 2007 **Charles University**, Faculty of Mathematics and Physics, Prague, Czech Rep. Study programme: Physics, Chemical Physics (5 year Masters programme) *Summa Cum Laude* Thesis: Non-elastic electron transport in molecular junctions Supervisor: Martin Čížek
Honors and Awards	2013: Second poster prize at the ISTCP-VIII conference

2012: Second place in JČMF Martin Odehnal's competition for young physicists
2010: Publication Prize of the UCL Chemistry Department
2009: Thomas Young Centre Junior Research Fellowship
2003–2007: Scholarship for excellent study results

Grants

2011: PhD+ Postdoctoral Fellowship
A competitive grant awarded to continue and extend the work started during PhD. Total budget ∼30.000£.

Membership

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

Referee for

Physical Review Letters, Physical Review B, Journal of Chemical Physics,
Journal of Physical Chemistry, Journal of Physics: Condensed Matter,
Physica Status Solidi.

Research interests

Development, implementation, and application of methods for description of weak interactions within density functional theory and post-Hartree–Fock approaches.
Methods for accurate description of electronic and structural properties of condensed systems.
Understanding connections between density functional theory, many-body perturbation theory, and post-Hartree–Fock methods.

Publications

25 publications in peer-reviewed journals.
1125 citations (including self-citations, according to Web of Science (WoS)).
ResearcherID: D-8926-2011.
H-index = 12.

Most important publications (most recent first):

J. Klimeš, M. Kaltak and G. Kresse: *Predictive GW calculations using plane waves and pseudopotentials*, Phys. Rev. B **90**, 075125 (2014).
Development of correction schemes for basis set incompleteness error of correlated methods within plane-wave basis set. Reference quality quasi-particle calculations within the *GW* approximation to the self-energy.
Selected as "Editor's suggestion".

J. Klimeš and A. Michaelides: *Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory*, J. Chem. Phys. **137**, 120901 (2012).
Invited review article describing the recent developments and future perspectives of dispersion corrected DFT methods.

J. Klimeš, D. R. Bowler, and A. Michaelides: *Van der Waals density functionals applied to solids*, Phys. Rev. B **83**, 195131 (2011).
Study of the performance of different van der Waals density functionals for "hard" solids.

J. Carrasco, B. Santra, **J. Klimeš**, and A. Michaelides: *To wet or not to wet? Dispersion forces tip the balance for water-ice on metals*, Phys. Rev. Lett. **106**, 026101 (2011).
Application of dispersion corrected DFT to the problem of incorrect relative description of binding of water on surfaces and in water ice. I performed some of the calculations

and guided colleagues with the set-up of the vdW-DF scheme and analysed the results.

B. Santra, **J. Klimeš**, D. Alfè, A. Tkatchenko, B. Slater, A. Michaelides, R. Car, and M. Scheffler: *Hydrogen bonds and van der Waals forces in ice at ambient and high pressures*, Phys. Rev. Lett. **107**, 185701 (2011).
Study of high pressure water ice phases using dispersion corrected DFT. I performed some of the calculations that used the vdW-DF scheme.

J. Klimeš, D. R. Bowler, and A. Michaelides: *Chemical accuracy for the van der Waals density functional*, J. Phys.: Cond. Mat. **22**, 022201 (2010).
Proposal of improvement of the van der Waals density functional of Langreth and Lundqvist and coworkers and application of the improved functional to different systems.
Selected as one of the "Highlights of 2010" articles in J. Phys.: Cond. Mat.

CONFERENCE PRESENTATIONS

Invited oral presentation:

J. Klimeš, A. Michaelides, *Van der Waals density functional applied to gas phase clusters and solid systems*
CECAM Meeting, Lausanne, Switzerland, October 2012.

8 contributed oral presentations at international conferences.

8 posters at international conferences, including:

J. Klimeš, A. Grüneis, G. Kresse,
Acceleration of basis set convergence of ACFDT-RPA and MP2 correlation energies using the effective energy techniques. ISTCP-VIII, Budapest, Hungary, August 2013.
Awarded second poster prize.

OUTREACH

Organiser of Michaelides' group stand at the Royal Society Summer Science Exhibition 2010. Specifically, I was responsible for the development of the web interface to the HEC-ToR supercomputer which enabled members of the public to run real time simulations on the country's biggest supercomputer. Also I was the impersonator of the George screen character for a set of short educational movies for the public which are available on YouTube.

Organiser of M&M magazine, a competition in Maths, Physics, and Informatics for high school students, 2002–2004.

LANGUAGE SKILLS

Czech (native), English (fluent), German (intermediate), basics of French.

INTERESTS

Mountaineering, Music, Photography.