



CONTACT INFORMATION

Jaap Kroes
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Tel: (+31) 683 70 56 85
Born: 2 Dec 1984, Arnhem

EDUCATION

Ecole Polytechnique Fédérale de Lausanne, Switzerland **Dec 2014**

Ph.D., EPFL – Computational Chemical Physics on the Nanoscale (C3PN)

- Thesis under supervision of Professor **W. Andreoni**
Carbon Nanotubes: Adsorption, Point Defects and Structural Deformation from Quantum and Classical Simulations

Radboud University, Nijmegen, Netherlands **June 2010**

M.Sc. (cum laude), Physics and Astronomy

- Thesis under supervision of Professor **A. Fasolino**:
Graphene Nanoribbons and Edge Reconstructions

B.Sc., Physics and Astronomy, **June 2008**

WORK EXPERIENCE

Postdoc, Radboud University, Netherlands **Apr 2015 – Apr 2017**

Postdoc, EPFL, Switzerland **Oct 2014 – Mar 2015**

IBM Zurich Research Lab, Rüschlikon, Switzerland **Apr 2012 – Apr 2014**

Teaching Assistance:

- Quantum Chemistry (RU) **autumn 2015**
- General Physics I (EPFL) **autumn 2013**
- Numerical Physics (EPFL) **autumn 2011 – spring 2013**
- Mathematical Methods in Physics (EPFL) **autumn 2011**
- Analytical Mechanics (EPFL) **spring 2011**
- Physics Labs for Biologists (EPFL) **autumn 2010**
- Biophysics (RU) **autumn 2009**
- Probability Theory (RU) **autumn 2006**

OTHER SKILLS

Languages

Dutch (native)
English (excellent)
French (excellent)
German (basic understanding)

Programming languages

Python, C(++), Fortran(77,90), HTML, CSS, shell scripting (bash, AWK)

List of Publications

- J.M.H. Kroes, A. Fasolino, M.I. Katsnelson, Energetics, barriers and vibrational spectra of partially and fully hydrogenated hexagonal boron nitride, *Phys. Chem. Chem. Phys.* 18, 19359 **2016**
- J.M.H. Kroes, F. Pietrucci, W. Andreoni, K. Chikkadi, C. Roman, C. Hierold, The response of single-walled carbon nanotubes to NO₂ and the search for a long-living adsorbed species, *Appl. Phys. Lett.* 108, **2016**
- J.M.H. Kroes, F. Pietrucci, A. van Duin, W. Andreoni, Atom Vacancies on a Carbon Nanotube: To What Extent Can We Simulate their Effects?, *J. Chem. Theory Comp.* 11, 3393 **2015**
- J.M.H. Kroes, F. Pietrucci, A. Curioni, and W. Andreoni, Characterizing and Understanding Divalent Adsorbates on Carbon Nanotubes with Ab-Initio and Classical Approaches: Size, Chirality and Coverage Effects, *J. Chem. Theory Comput.* 10, 4672 **2014**
- J.M.H. Kroes, F. Pietrucci, A. Curioni, R. Jaafar, O. Gröning, and W. Andreoni, Atomic Oxygen Chemisorption on Carbon Nanotubes Revisited with Theory and Experiment, *J. Phys. Chem. C* 117, 1948 **2013**
- W. Andreoni, A. Curioni, J. M. H. Kroes, F. Pietrucci and O. Gröning, Exohedral Hydrogen Chemisorption on a Carbon Nanotube: The Clustering Effect, *J. Phys. Chem. C* 116, 269 **2012**
- J.M.H. Kroes, M.A. Akhukhov, J.H. Los, N. Pineau, A. Fasolino, Mechanism and free-energy barrier of the type-57 reconstruction of the zigzag edge of graphene, *Phys. Rev. B* 83, 165411 **2011**

List of Presentations

- “Physics@Veldhoven”, NWO meeting Veldhoven; Jan 17–18 **2017 (talk)**
- “Materials Research Society Spring Meeting 2014”, San Francisco, United States; Apr 21–25 **2014 (talk)**
- “Nano-Tera.ch Annual Meeting 2013” in Bern, Switzerland; May 30–31 **2013 (poster)**
- “Energy from the Sun: Computational Chemists and Physicists Take up the Challenge” conference, Italy; Sept 10–14 **2012 (poster)**
- “Nano-Tera.ch Annual Meeting 2012” Meeting in Zurich, Switzerland; Apr 26–27 **2012 (poster)**
- “Chemical and Topological Functionalization of Graphitic Surfaces: Open Challenges for Computational Modeling”, workshop; Lausanne, Switzerland; April 23–25 **2012 (poster)**
- “Towards Reality in Nanoscale Materials V”, workshop in Levi, Finland; Feb 20–22 **2012 (poster)**
- “Trends in Nanotechnology 2011”, conference; Tenerife (Spain), Nov 21–25 **2011 (poster)**
- “DFT and Beyond: Hands-on Tutorial Workshop 2011 on Ab Initio Molecular Simulations: Toward a First-Principles Understanding of Materials Properties and Functions”, workshop; Berlin, Germany; July 12–21 **2011 (poster)**
- “Towards Reality in Nanoscale Materials '10”, workshop; Levi, Finland **2010 (poster)**