KRISTOF BAL

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PROFILE

I am a researcher interested in the development of advanced simulation techniques and their application to challenging problems in the chemical sciences. I also enjoy sharing my interests through teaching, coaching of students, and scientific communication to a wider audience.

RESEARCH EXPERIENCE

University of Antwerp 2018–present
Postdoctoral Researcher

University of Antwerp 2014–18
PhD Researcher
Supervisor: Erik C. Neyts. Funded by an FWO Fellowship (Aspirant).

ETH Zurich and USI Lugano 2017
Visiting Researcher
6 week stay with prof. Michele Parrinello in Lugano

EDUCATION

University of Antwerp 2014–18
PhD in Science: Chemistry

University of Antwerp 2012–14
MSc. Chemistry, *summa cum laude*
Thesis in the PLASMANT research group, supervisor: Erik C. Neyts

University of Antwerp 2009–12
BSc. Chemistry, *summa cum laude*

SKILLS & EXPERTISE

- **Computational chemistry:** molecular dynamics, Monte Carlo methods, free energy methods, enhanced sampling techniques (metadynamics, hyperdynamics, and own developments), density functional theory from single molecules to condensed systems.
- **Methodology development:** Derivation, implementation and application of new atomistic simulation algorithms. Development of new approaches to analyze experimental data.
- **Computing:** Windows/Linux, programming (C/C++, Fortran, Python, Unix shell scripting), HPC environments, scientific software (CP2K, LAMMPS, Gaussian, PLUMED), standard tools (office packages, LaTeX, multimedia, etc.).

- **Coaching:** Co-supervised 4 bachelor thesis students and aspects of 5 PhD projects.
- **Industry collaboration:** Implementation of my simulation methods by Software for Chemistry & Materials in their commercial packages. Performed DFT calculations to support experimental observations and industrial methodologies developed by imec.
- **Languages:** Dutch (native), English (excellent), German (excellent), French (basic).

AWARDS

- Semifinalist of the **Flemish PhD Cup** (16 selections out of 73 submissions). Selected by a panel consisting of science journalists and academics of the Jonge Academie. (2019)
- **PSST Highlights of 2018**. The article "Effect of plasma-induced surface charging on catalytic processes: application to CO_2 activation" was selected as one of the best papers published in the journal in 2018. Awarded by the editors of *Plasma Sources Science and Technology*. (2019)
- **Best poster award** (first prize out of ~200 posters) at the *23rd International Symposium on Plasma Chemistry* (ISPC23), Montreal, Canada. Awarded by IPCS/IOP. (2017)
- **JCP Editors' Choice** for the article "On the time scale associated with Monte Carlo simulations." Awarded by the editors of *The Journal of Chemical Physics*. (2015)
- **KVCV award.** For the most meritorious Chemistry student graduating from the University of Antwerp. Awarded by the Royal Flemish Chemical Society (KVCV). (2014)
- Oxford University Press **Achievement in Chemistry Prize**. For the best Bachelor student in Chemistry. (2010)

GRANTS

- **FWO junior postdoctoral fellowship** (3 years). (2019)
- **FWO travel grant** for participation in a conference abroad. Attendance of the joint *XXXIV ICPIG & ICRP-10* conferences, Sapporo, Japan. (2019)
- **FWO travel grant** for a long stay abroad. Research visit to the ETH Zurich at Lugano. (2017)
- **FWO PhD fellowship** (2 + 2 years). (2014)

SCIENCE COMMUNICATION & OUTREACH

- Participated in the **PRESS>SPEAK** science communication event of the University of Antwerp and created a video for the *Science Figured Out* web site based on the talk. (2020)
- Participated in the **Flemish PhD Cup**. 3-minute pitch about my PhD research for a general audience and an article on the *Eos* science blog, entitled "Chemicus zonder reageerbuis." (2019)
- Participated in the **Wetenschapsbattle.** Presentation of my research to young children in elementary school (ages 6–12), entitled "Schadelijke gassen vangen met een computer." (2019)
- **Guest lecture at Go! Geel Atheneum** high school. Interactive presentation linking my research to chemical concepts taught in class, entitled "Computersimulaties van materie en chemische reacties." (2019)
- Volunteer science communication of the ***CurieuzeNeuzen* citizen science project**, organized by the University of Antwerp, *de Standaard*, and the Flanders Environment Agency (VMM). (2018)
- Crew member of **Wetenschapsforum.nl**. Responsible for news posting and answering science-related questions on the leading Dutch science-related message board. (2011–2014)

PUBLICATIONS

1. S. Fukuhara, K. M. Bal, E. C. Neyts & Y. Shibuta. Entropic and enthalpic factors determining the thermodynamics and kinetics of carbon segregation from transition metal nanoparticles. *Carbon*. In revision (2020).
2. K. M. Bal, S. Fukuhara, Y. Shibuta & E. C. Neyts. Free energy barriers from biased molecular dynamics simulations. *J. Chem. Phys.* In press (2020).
3. Y. Uytdenhouwen, K. M. Bal, E. C. Neyts, V. Meynen, P. Cool & A. Bogaerts. On the kinetics and equilibria of plasma-based dry reforming of methane. *Chem. Eng. J.* **405**, 126630 (2021).
4. A. Jafarzadeh, K. M. Bal, A. Bogaerts & E. C. Neyts, Activation of CO_2 on copper surfaces: The synergy between electric field, surface morphology, and excess electrons. *J. Phys. Chem. C* **124**, 6747–6755 (2020).
5. S. Fukuhara, K. M. Bal, E. C. Neyts & Y. Shibuta. Accelerated molecular dynamics simulation of large systems with parallel collective variable-driven hyperdynamics. *Comput. Mater. Sci.* **177**, 109581 (2020).
6. K. M. Bal, A. Bogaerts & E. C. Neyts. Ensemble-based molecular simulation of chemical reactions under vibrational nonequilibrium. *J. Phys. Chem. Lett.* **11**, 401–406 (2020).
7. Y. Uytdenhouwen, K. M. Bal, I. Michielsen, E. C. Neyts, V. Meynen, P. Cool & A. Bogaerts. How process parameters and packing materials tune chemical equilibrium and kinetics in plasma-based CO_2 conversion. *Chem. Eng. J.* **372**, 1253–1264 (2019).
8. A. Jafarzadeh, K. M. Bal, A. Bogaerts & E. C. Neyts. CO_2 activation on TiO_2-supported Cu_5 and Ni_5 nanoclusters: effect of plasma-induced surface charging. *J. Phys. Chem. C* **123**, 6516–6525 (2019).
9. K. M. Bal & E. C. Neyts. Overcoming old scaling relations and establishing new correlations in catalytic surface chemistry: combined effect of charging and doping. *J. Phys. Chem. C* **123**, 6141–6147 (2019).
10. D. U. B. Aussems, K. M. Bal, T. W. Morgan, M. C. M. van de Sanden & E. C. Neyts. Mechanisms of elementary hydrogen ion-surface interactions during multilayer graphene etching at high surface temperature as a function of flux. *Carbon* **137**, 527–532 (2018).
11. S. Huygh, A. Bogaerts, K. M. Bal & E. C. Neyts. The high coke resistance of a TiO_2 anatase (001) catalyst surface during dry reforming of methane. *J. Phys. Chem. C* **122**, 9389–9396 (2018).
12. K. M. Bal & E. C. Neyts. Modelling molecular adsorption on charged or polarized surfaces: a critical flaw in common approaches. *Phys. Chem. Chem. Phys.* **20**, 8456–8459 (2018).
13. K. M. Bal, S. Huygh, A. Bogaerts & E. C. Neyts. Effect of plasma-induced surface charging on catalytic processes: application to CO_2 activation. *Plasma Sources Sci. Technol.* **27**, 024001 (2018).
14. D. U. B. Aussems, K. M. Bal, T. W. Morgan, M. C. M. van de Sanden & E. C. Neyts. Atomistic simulations of graphite etching at realistic time scales. *Chem. Sci.* **8**, 7160–7168 (2017).
15. E. C. Neyts & K. M. Bal. Effect of electric fields on plasma catalytic hydrocarbon oxidation from atomistic simulations. *Plasma Process. Polym.* **14**, e1600158 (2017).
16. K. M. Bal, J. Cautereels & F. Blockhuys. Structures and spectroscopic properties of sulfur-nitrogen-pnictogen chains: $R_2P–N=S=N–PR_2$ and $R_2P–N=S=N–AsR_2$. *J. Mol. Struct.* **1132**, 102–108 (2017).
17. K. M. Bal & E. C. Neyts. Direct observation of realistic-temperature fuel combustion mechanisms in atomistic simulations. *Chem. Sci.* **7**, 5280–5286 (2016).
18. K. M. Bal & E. C. Neyts. Merging metadynamics into hyperdynamics: accelerated molecular simulations reaching time scales from microseconds to seconds. *J. Chem. Theory Comput.* **11**, 4545–4554 (2015).

19. K. M. Bal & E. C. Neyts. On the time scale associated with Monte Carlo simulations. *J. Chem. Phys.* **141**, 204104 (2014).
20. W. Somers, A. Bogaerts, A. C. T. van Duin, S. Huygh, K. M. Bal & E. C. Neyts. Temperature influence on the reactivity of plasma species on a nickel catalyst surface: An atomic scale study. *Catal. Today* **211**, 131–136 (2013).
21. E. C. Neyts, B. J. Thijsse, M. J. Mees, K. M. Bal & G. Pourtois. Establishing uniform acceptance in force biased Monte Carlo simulations. *J. Chem. Theory Comput.* **8**, 1865–1869 (2012).

INVITED SEMINARS

1. Long time scale atomistic simulations of large-scale transformations with collective variable-driven hyperdynamics. *Department of Computational Materials Design*, Max Planck Institute for Iron Research, Düsseldorf, Germany, December 10, 2018.
2. Atomistic simulations of large-scale chemical transformations with collective variable-based methods. *Institute of Computational Science*, ETH Zürich and Università della Svizzera italiana, Lugano, Switzerland, September 28, 2017.
3. Long time scale atomistic simulations of large reactive systems: from metadynamics to hyperdynamics (and back again). *Institute of Mineralogy, Materials Physics and Cosmochemistry*, Université Pierre et Marie Curie (Paris VI), Paris, France, June 19, 2017.

CONFERENCE PRESENTATIONS

1. New physicochemistry at the plasma–catalyst interface: Insights from atomistic modeling. Satellite symposium *Challenges in simulation of low-temperature plasma and its applications* at the joint *XXXIV ICPIG & ICRP-10* conferences, Sapporo, Japan, July 14–19, 2019. **(invited talk)**
2. Bottom-up disentanglement of plasma-catalytic effects from atomistic modeling. *2018 Plasma Processing Science Gordon Research Conference*, Bryant University, RI, USA, August 5–10, 2018. **(invited talk)**
3. Bottom-up disentanglement of plasma-catalytic effects from atomistic modeling. *2018 Plasma Processing Science Gordon Research Seminar*, Bryant University, RI, USA, August 4–5, 2018. **(poster presentation)**
4. Atomistic modeling of carbon nanostructures: challenges and opportunities. *2018 EMRS Spring Meeting*, Strasbourg, France, June 18–22, 2018. **(invited talk)**
5. From microscopic simulations to macroscopic time scales in reactive MD. *ADF Developer Meeting 2018*, Software for Chemistry & Materials (SCM), Vrije Universiteit Amsterdam, The Netherlands, March 26–29, 2018. **(invited talk)**
6. Effect of plasma surface charging on catalytic activation of CO2: Fundamental insights from quantum chemical modeling. *23rd International Symposium on Plasma Chemistry*, Montreal, Canada. July 30–August 4, 2017. **(poster and oral flash presentation)**
7. Effect of plasma surface charging on the catalytic decomposition of carbon dioxide. *iPlasmaNano VIII* conference, University of Antwerp, Belgium, July 3–6, 2017. **(poster presentation)**
8. Bridging time scales in atomistic simulations: from classical models to density functional theory. *VSC Users Day*, Royal Flemish Academy of Belgium for Science and the Arts, Brussels, Belgium, June 2, 2017. **(poster and oral flash presentation)**
9. Collective variable-driven hyperdynamics: atomistic simulations of complex processes reaching long time scales. *Computational Molecular Science* conference, University of Warwick, UK, March 19–22, 2017. **(poster presentation)**

10. Flexible accelerated molecular dynamics with a hybrid metadynamics/hyperdynamics method. *Bridging-Time Scale Techniques and their Applications in Atomistic Computational Science* focus workshop, Max Planck Institute for the Physics of Complex Systems in Dresden, Germany, September 12–15, 2016. **(oral presentation)**
11. Flexible accelerated molecular dynamics with a hybrid metadynamics/hyperdynamics method. *AIP Publishing Horizons Future of Chemical Physics* conference, University of Oxford, UK, August 31–September 2, 2016. **(poster presentation)**
12. The time scale associated with Monte Carlo simulations. *Spring School on Computational Tools for Materials Science*, Ghent University, Belgium, April 13–17, 2015. **(poster presentation)**

TEACHING EXPERIENCE

- **General Chemistry** (*Chemie I*, 1001WETCHE): Teaching assistant in the practice sessions, for Prof. E. Neyts. (fall 2016)
- **Organic Chemistry** (*Organische chemie m.i.v. labovaardigheden*, 1043FBDBMW): Teaching assistant in the practice and/or lab sessions for Prof. F. Lemière. (spring 2015–2019)
- **General Chemistry** (*Algemene chemie m.i.v. labovaardigheden*, 1042FBDBMW): Teaching assistant in the lab sessions, for Prof. F. Blockhuys. (fall 2014–2019)
- **Refresher Courses Chemistry** (*Overbruggingsonderwijs Chemie*): Refresher courses chemistry for freshmen Biology, Biomedical Sciences and Veterinary Medicine. (September 2012 & 2013)