Curriculum Vitae Dr. Dr. Danny E. P. Vanpoucke

Current Affiliation:

Maastricht University
Institute for Materials Research (IMO)
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dannyvanpoucke@gmail.com
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Work Experience

2020–2021: **guest professor**
Hasselt University

At the department of Chemistry of the UHasselt. (Belgium)
Contributing to the development of a new master's program at UHasselt.

2020–2021: **Lecturer**
Hasselt University

At the department of Physics of the UHasselt. (Belgium)

Teaching experience:
Lecturer : Statistical Physics

2019–2020: **postdoc**
Maastricht University

In the Aachen–Maastricht Institute for Biobased Materials (AMIBM) with Prof. Dr. K. Bernaerts (AMIBM) and Prof. Dr. S. Mehrkanoon (DKE), at the UMaastricht. (The Netherlands)
Developing a Machine-Learning framework for small (experimental) data sets.

2017–2019: **postdoc**
Hasselt University

In the Wide Bandgap Materials group (WBGM) of Prof. Dr. K. Haenen, at the UHasselt. (Belgium)

Teaching experience:
Teaching assistant : Biophysics
Lecturer : Functional Molecular Modeling

Coordinator/Lecturer : Experimental Techniques
Promoter Bachelor projects:
- "*Benchmarking DFT-functionals for periodic C-based materials*"
- "*Are there atoms in molecules*"

2014–2017: **FWO postdoctoral Fellow**
Ghent University and Hasselt University

In the Wide Bandgap Materials group (WBGM) of Prof. Dr. K. Haenen, at the UHasselt. (Belgium)

Teaching experience:
Teaching assistant : Biophysics
Co-lecturer : Functional Molecular Modeling
Promoter Bachelor projects:
- "*Applied Phonons – Vibrational properties of Metal-Organic Frameworks*"
- "*Germanium-Vacancy Complexes in Diamond*"

In the Center for Molecular Modeling (CMM) of Prof. Dr. Ir. V. Van Speybroeck, at Ghent University. (Belgium)

Teaching experience:
Counselor of Master-thesis: "*Combined theoretical-experimental study of chromium doped zinc gallate phosphor.*"

2013–2014: **postdoc**
Ghent University

In the Center for Molecular Modeling (CMM) of Prof. Dr. Ir. V. Van Speybroeck, at Ghent University. (Belgium)

nov-dec 2012: **projectworker PMGE**
Ghent University

At the Department of Administrative Affairs, supervising of the roll-out of the PMGE project:
- The introduction of new research groups and departments to the project
- Monitoring, supervision, and providing support for previously introduced groups.

2009–2012: **Ph.D./postdoc**
Ghent University

In the SCRiPTS group of Prof. Dr. I. Van Driessche, part of the Department of Inorganic and Physical Chemistry, at the Ghent University. (Belgium)

Teaching experience:
Provided working classes for the courses:
- Quantum chemistry
- Chemical bond
Supervision of Bachelor project: "*Undecided electrons in ab initio calculations : What happens if the f electron in CeO_2 is uncertain whether to join in or not.*"

2005–2009: **Research assistant (OIO)**
Foundation for Fundamental Research on Matter, and
University of Twente

In the Computational Materials Science group of Prof. Dr. P. J. Kelly under supervision of Dr. G. Brocks, at the university of Twente. (The Netherlands)

Teaching experience:
Provided working classes for the course “Introduction to Quantum Mechanics”

2004–2005: **Interim Teacher Physics/Chemistry**
KTA de Merodelei, Turnhout, Belgium

2003: **Tutor**
Memento-Mementec-Memodi, Ghent, Belgium

Education/Degrees

2009–2012: **Ph.D. in Chemistry**
Ghent University

Ph.D. Thesis: Investigation of tunable buffer layers for coated superconductors: from solid state physics to quantum chemistry.
Defence: October 5^{th}, 2012
Promoter: Prof. Dr. I. Van Driessche
Co-Promoter: Prof. Dr. P. Bultinck

2005–2009: **Ph.D. in Physics**
University of Twente, The Netherlands

Ph.D. Thesis: *Ab Initio Study of Pt Induced Nanowires on Ge(001)*
Defence: September 11^{th}, 2009
Promoters: Prof. Dr. P. J. Kelly and Dr. G. Brocks

1998–2004: **B. Sc. and M.Sc. Physics**
Ghent University, Belgium

Master thesis: *Bose-Einstein condensation in exactly solvable systems (in Dutch)*
Promoter: Dr. S. Rombouts
Supervisor: Ir. L. Pollet

Honors and Awards

- First prize at Casting Keynotes at TEDxUHasselt (2019)
- Cover Image of Crystal Engineering Communication Vol 17, Issue 45, page 8565, 2015 doi:10.1039/C5CE90198G
- Cover Image of Journal of Computational Chemistry Vol 34, Issue 5, pages i-ii, 2013 doi:10.1002/jcc.23239
- Young speakers award at the Belgian Physical Society annual general meeting 2011
- Finalist in the ”Science as art competition” of the 2009 Materials Research Society (MRS) Spring meeting, San Fransisco, USA, april 13th-17th 2009

Grants

2019 Joined Ph.D. Fellowship UNamur-UHasselt for Emerick Guillaume: *“Growth and doping of graphene and diamond by means of first-principles calculations”*

2014 FWO grant postdoctoral fellowship: *“Elucidating the role of 1-dimensional metal-oxide chains in the physical and chemical properties of porous metal-organic frameworks by means of density functional theory calculations”*

2013-2018 10 HPC-projects: 20.9 M CPU hours (519k€), **Flemish Supercomputer Center (VSC)**, Belgium

- 2021: 3721 node-days for the project:*"Growth of Phosphorous doped diamond: dynamics, bonding and charge transfer, Part II"*
- 2020: 3000 node-days for the project:*"Growth of Phosphorous doped diamond: dynamics, bonding and charge transfer"*
- 2019: 3150 node-days for the project:*"Si based luminescent centres in diamond"*
- 2019: 3050 node-days for the project:*"Elucidating the surface-dopant interactions of the negative electron affinity diamond surfaces"*
- 2018: 3069 node-days for the project:*"New luminescent centers in diamond: Eu and Ge single centers"*
- 2017: 3100 node-days for the project:*"Breathing behavior of flexible mixed metal Metal-Organic Frameworks."*
- 2016: 4970 node-days for the project:*"Breathing behavior of flexible Metal-Organic Frameworks with MIL-47/53 topology"*
- 2015: 2905 node-days for the project:*"The electronic structure of functionalized luminescent Metal-Organic Frameworks"*
- 2014: 4725 node-days for the project:*"The electronic and magnetic structure of Breathing Metal-Organic Frameworks"*
- 2013: 8272 node-days for the project:*"Structural and atomic charge evolution in the breathing behavior of Metal Organic Frameworks"*

2009 Granted 20 000 hours CPU time by the **Stichting Nationale Computer Faciliteiten (NCF)** on the Dutch Huygens supercomputer, for the project:*"Ab initio modeling of metallic monatomic nanowire arrays on Ge(001)"*

Software

VASP, sk-learn
Fortran95, Fortran2003, Python, Delphi, Pascal, Java, C++(basics)
bash script, HTML, CSS, Java script
LaTeX 2$_\varepsilon$, MS Office, xmgrace, Maple, gnuplot, Jasc Paint Shop

Professional Membership

Belgian Physical Society (BPS)
European Physical Society (EPS)
Materials Research Society (MRS)

Science Communication

2021 TEDxUHasselt lecture: "The Virtual Lab"
2019 Lecture at Universiteit van Vlaanderen
2019 Casting Keynotes (selection for TEDxUHassselt): The Virual Lab (First prize)
2019 Plenary session of the summer school: Let's Talk Science (UAntwerpen)
2018 Wetenschap Uitgedokterd
2018 de Wetenschapsbattle
2018-... EOS wetenschap blog [Dutch]
2015-... Blog on personal website [English]

Language Skills

Dutch (native speaker), English (fluent), French (good), German (basics), Latin (reading)

Interests

Travel, salsa, books, games, programming

Scientific Appendix

List of Publications

A1 Publications

[1] *Impact of Methane Concentration on Surface Morphology and Boron Incorporation of Heavily Boron-doped Single Crystal Diamond Layers*
Rozita Rouzbahani, Shannon S. Nicley, Danny E. P. Vanpoucke, Fernando Lloret, Paulius Pobedinskas, Daniel Araujo, and Ken Haenen
Carbon **172**, 463-473 (2021).

[2] *Small Data Materials Design with Machine Learning: When the Average Model Knows Best*
Danny E. P. Vanpoucke, Onno S. J. van Knippenberg, Ko Hermans, Katrien V. Bernaerts, and Siamak Mehrkanoon
J. Appl. Phys. **128**, 054901 (2020). **[Featured Article]**

[3] *Partitioning the vibrational spectrum: Fingerprinting defects in solids*
Danny E. P. Vanpoucke
Comput. Mater. Sci. **181**, 109736 (2020).

[4] *Influence of diamond crystal orientation on the interaction with biological matter*
Viraj Damle, Kaiqi Wu, Oreste De Luca, Natalia Ortí-Casañ, Neda Norouzi, Aryan Morita, Joop de Vries, Hans Kaper, Inge Zuhorn, Ulrich Eisel, Danny E.P. Vanpoucke, Petra Rudolf, and Romana Schirhagl
Carbon **162**, 1-12 (2020).

[5] *UV-Curable Biobased Polyacrylates Based on a Multifunctional 2 Monomer Derived from Furfural*
Jules Stouten, Danny E. P. Vanpoucke, Guy Van Assche, and Katrien V. Bernaerts
Macromolecules **53(4)**, 1388-1404 (2020).

[6] *Investigation of structural, electronic and magnetic properties of breathing metal–organic framework MIL-47(Mn): a first principles approach*
Mohammadreza Hosseini, Danny E.P. Vanpoucke, Paolo Giannozzi, Masoud Berahman, Nasser Hadipour
RSC Adv. **10**, 4786-4794 (2020).

[7] *Can Europium Atoms form Luminescent Centres in Diamond: A combined Theoretical–Experimental Study*
Danny E. P. Vanpoucke, Shannon S. Nicley, Jorne Raymakers, Wouter Maes, and Ken Haenen
Diam. Relat. Mater. **94**, 233-241 (2019).

[8] *Synthesis, characterization and thermodynamic stability of nanostructured ε-iron carbonitride powder prepared by a solid-state mechanochemical route*
Seyyed Amin Rounaghi, Danny E. P. Vanpoucke, Elaheh Esmaeili, Sergio Scudino, and Jürgen Eckert
J. Alloys. Compd. **778**, 327-336 (2019).

[9] *Predicting Partial Atomic Charges in Siliceous Zeolites*
Jarod J. Wolffis, Danny E. P. Vanpoucke, Amit Sharma, Keith V. Lawler, and Paul M. Forster
Microporous and Mesoporous Materials **277**, 184-196 (2019).

[10] *Revisiting the Neutral C-Vacancy in Diamond: Localization of Electrons through DFT+U*
Danny E. P. Vanpoucke and Ken Haenen
Diam. Relat. Mater. **79**, 60-69 (2017).

[11] *A combined experimental and theoretical investigation of the Al-Melamine reactive milling system: a mechanistic study towards AlN-based ceramics*
Seyyed Amin Rounaghi, Danny E. P. Vanpoucke, Hossein Eshghi, Sergio Scudino, Elaheh Esmaeili, Steffen Oswald, and Jürgen Eckert
J. Alloys Compd. **729**, 240-248 (2017).

[12] *Mechanochemical synthesis of nanostructured metal nitrides, carbonitrides and carbon nitride: A combined theoretical and experimental study*
Seyyed Amin Rounaghi, Danny E. P. Vanpoucke, Hossein Eshghi, Sergio Scudino, Elaheh Esmaeili, Steffen Oswald, and Jürgen Eckert
Phys. Chem. Chem. Phys. **19**, 12414-12424 (2017).

[13] *Linker Functionalization in MIL-47(V)-R Metal-Organic Frameworks: Understanding the Electronic Structure*
Danny E. P. Vanpoucke
J. Phys. Chem. C **121(14)**, 8014-8022 (2017).

[14] *Mechanochemical route to the synthesis of nanostructured Aluminium nitride*
Seyyed Amin Rounaghi, Hossein Eshghi, Sergio Scudino, Anastasia Vyalikh, Danny E. P. Vanpoucke, Wolfgang Gruner, Steffen Oswald, Ali-Reza Kiani-Rashid, Mohsen Samadi-Khoshkhoo, Ulrich Scheler, and Jürgen Eckert
Scientific Reports **6**, 33375 (2016).

[15] *First-Principles Study of Antisite Defect Configurations in $ZnGa_2O_4$:Cr Persistent Phosphors*
Arthur De Vos, Kurt Lejaeghere, Danny E.P. Vanpoucke, Jonas J. Joos, Philippe F. Smet, and Karen Hemelsoet
Inorg. Chem. **55(5)**, 2402–2412 (2016).

[16] *Understanding intrinsic light absorption properties of UiO-66 frameworks: A combined theoretical and experimental study*
Kevin Hendrickx, Danny E.P. Vanpoucke, Karen Leus, Kurt Lejaeghere, Andy Van Yperen-De Deyne, Veronique Van Speybroeck, Pascal Van Der Voort, and Karen Hemelsoet
Inorg. Chem. **54(22)**, 10701-10710 (2015).

[17] *Mechanical Properties from Periodic Plane Wave Quantum Mechanical Codes: The Challenge of the Flexible Nanoporous MIL-47(V) Framework*
Danny E. P. Vanpoucke, Kurt Lejaeghere, Veronique Van Speybroeck, Michel Waroquier, and An Ghysels
J. Phys. Chem. C **119(41)**, 23752-23766 (2015).

[18] *Fine-tuning the theoretically predicted structure of MIL-47(V) with the aid of powder X-ray diffraction*
Thomas Bogaerts, Louis Vanduyfhuys, Danny E.P. Vanpoucke, Jelle Wieme, Michel Waroquier, Pascal Van Der Voort, and Veronique Van Speybroeck,
Cryst. Eng. Comm. **17(45)**, 8612-8622 (2015).

[19] *A Flexible Photoactive Titanium Metal-Organic Framework Based on a $[Ti_3^{IV}(\mu_3\text{-}O)(O)_2(COO)_6]$ Cluster*
Bart Bueken, Frederik Vermoortele, Danny E. P. Vanpoucke, Helge Reinsch, Chih-Chin Tsou, Pieterjan Valvekens, Trees De Baerdemaeker, Rob Ameloot, Christine E. A. Kirschhock, Veronique Van Speybroeck, James M. Mayer and Dirk De Vos,
Angew. Chem. Int. Ed. **54(47)**, 13912-13917 (2015).

[20] *Convergence of Atomic Charges with the Size of the Enzymatic Environment*
Danny E. P. Vanpoucke, Julianna Oláh, Frank De Proft, Veronique Van Speybroeck, and Goedele

Roos
J. Chem. Inf. Model. **55**(**3**), 564-571 (2015).

[21] *Comment on "Europium doping induced symmetry deviation and its impact on the second harmonic generation of doped ZnO nanowires."*
Danny E. P. Vanpoucke
Nanotechnology **25**(**45**), 458001 (2014).

[22] *Quasi-1D physics in metal-organic frameworks: MIL-47(V) from first principles*
Danny E. P. Vanpoucke, Jan W. Jaeken, Stijn De Baerdemacker, Kurt Lejaeghere, and Veronique Van Speybroeck
Beilstein J. Nanotechnol. **5**, 1738–1748 (2014).

[23] *Aliovalent Doping of CeO_2: DFT study of oxidation state and Vacancy effects*
Danny E. P. Vanpoucke, Patrick Bultinck, Stefaan Cottenier, Veronique Van Speybroeck, and Isabel Van Driessche
J. Mater. Chem. A **2**, 13723–13737 (2014).

[24] *Rationality: A Social-Epistemology Perspective*
Sylvia Wenmackers, Danny E. P. Vanpoucke, and Igor Douven
Front. Psychol. **5**, 581 (2014).

[25] *Modeling 1D structures on semiconductor surfaces: Synergy of theory and experiment*
Danny E. P. Vanpoucke
J. Phys.: Condensed Matter, **26**(**13**), 133001 (2014). (Invited Topical Review)

[26] *Tetravalent Doping of CeO_2: The impact of valence electron character on group IV dopant influence*
Danny E. P. Vanpoucke, Stefaan Cottenier, Veronique Van Speybroeck, Isabel Van Driessche, and Patrick Bultinck
J. Am. Ceram. Soc. **97**(**1**), 258-266 (2014).

[27] *New Functionalized Metal-Organic Frameworks MIL-47-X (X = -Cl, -Br, -CH_3, -CF_3, -OH, -OCH_3): Synthesis, Characterization and CO_2 Adsorption Properties*
Shyam Biswas, Danny E. P. Vanpoucke, Toon Verstraelen, Matthias Vandichel, Sarah Couck, Karen Leus, Ying-Ya Liu, Michel Waroquier, Veronique Van Speybroeck, Joeri Denayer, and Pascal Van Der Voort
J. Phys. Chem. C **117**(**44**), 22784-22796 (2013).

[28] *Reply to 'Comment on "Extending Hirshfeld-I to bulk and periodic materials" '*
D. E. P. Vanpoucke, I. Van Driessche, and P. Bultinck
J. Comput. Chem. **34**, 422-427 (2013).

[29] *Extending Hirshfeld-I to bulk and periodic materials*
D. E. P. Vanpoucke, P. Bultinck, and I. Van Driessche
J. Comput. Chem. **34**, 405-417 (2013).

[30] *Aqueous CSD approach for the growth of novel, lattice-tuned $La_xCe_{1-x}O_\delta$ epitaxial layers*
Vyshnavi Narayanan, Petra Lommens, Klaartje De Buysser, Danny E.P. Vanpoucke, Ruben Huehne, Leopoldo Molina, Gustaaf Van Tendeloo , Pascal Van Der Voort, Isabel Van Driessche
J. Materials Chem. **22**, 8476 (2012).

[31] *Models and simulations in material science: two cases without error bars*
Sylvia Wenmackers and Danny E. P. Vanpoucke
Statistica Neerlandica **66**, 339-355 (2012).

[32] *Tuning of CeO_2 buffer layers for coated superconductors through doping*
Danny E. P. Vanpoucke, Stefaan Cottenier, Veronique Van Speybroeck, Patrick Bultinck, and Isabel

Van Driessche
Appl. Surf. Sci. **260**, 32-35 (2012).

[33] *Probability of inconsistencies in theory revision, A multi-agent model for updating logically interconnected beliefs under bounded confidence*
S. Wenmackers, D. E. P. Vanpoucke, and I. Douven
Eur. Phys. J. B **85**, 44 (2012).

[34] *Density functional theory study of $La_2Ce_2O_7$: disordered fluorite vs pyrochlore structure*
Danny E. P. Vanpoucke, Patrick Bultinck, Stefaan Cottenier, Veronique Van Speybroeck, and Isabel Van Driessche
Phys. Rev. **B 84**, 054110 (2011).

[35] *CO adsorption on Pt induced Ge nanowires*
D. E. P. Vanpoucke and G. Brocks
Phys. Rev. **B 81**, 235434 (2010).

[36] *Pt-induced nanowires on Ge(001): A density functional theory study*
D. E. P. Vanpoucke and G. Brocks
Phys. Rev. **B 81**, 085410 (2010).

[37] *Density functional theory study of Pt-induced Ge(001) reconstructions*
D. E. P. Vanpoucke and G. Brocks
Phys. Rev. **B 81**, 035333 (2010).

[38] *Formation of Pt-induced Ge atomic nanowires on Pt/Ge(001): A density functional theory study*
D. E. P. Vanpoucke and G. Brocks
Phys. Rev. **B 77**, 241308(R) (2008).

non-A1 Publications

[1] *Computational Materials Science: Where Theory Meets Experiments.*
Danny E. P. Vanpoucke
ICACC 2015 conference proceeding, Developments in Strategic Ceramic Materials: Ceramic Engineering and Science Proceedings, **Vol. 36(8)**, 323-334 (2016), ISBN: 978-1-119-21173-0.

[2] *Doping of CeO_2 as a Tunable Buffer Layer for Coated Superconductors: A DFT Study of Mechanical and Electronic Properties.*
Danny E. P. Vanpoucke
ICACC 2015 conference proceeding, Developments in Strategic Ceramic Materials: Ceramic Engineering and Science Proceedings, **Vol. 36(8)**, 169-177 (2016), ISBN: 978-1-119-21173-0.

[3] *Pt Nanowires on Ge(001): Sheep in Wolf's Clothing?*
Danny E. P. Vanpoucke
Belgian Physical Society Magazine 3, 11-16 (2011) (Feature Article).

[4] *The formation of self-assembled nanowire arrays on Ge(001): a DFT study of platinum induced nanowire arrays* in *Computational Nanoscience – How to Exploit Synergy between Predictive Simulations and Experiment.*
D. E. P. Vanpoucke and G. Brocks
(Mater. Res. Soc. Symp. Proc. **Volume 1177E**, Warrendale, PA, 2009),1177-Z03-09.

Ph.D. Theses and Book Chapter

[1] *Book-Chapter:"Computational Chemistry Experiment Possibilities"*
Bartłomiej M. Szyja and Danny E. P. Vanpoucke

In V. Blay, L. F. Bobadilla, & A. Cabrera (Eds.), *Zeolites and metal-organic frameworks. From lab to industry.* (pp. 235-264), Amsterdam University Press, (2018).

[2] *Investigation of tunable buffer layers for coated superconductors*
D. E. P. Vanpoucke
Ph.D. Thesis Ghent University, Belgium (2012).

[3] *Ab Initio study of Pt Induced Nanowires on Ge(001)*
D. E. P. Vanpoucke
Ph.D. Thesis University of Twente, The Netherlands, ISBN: 978-90-365-2873-3 (2009).

In preparation

[1] *On the role of water in molecular crystals. THz vibrational spectroscopy analysis*
Sergey Mitryukovskiy, Danny E. P. Vanpoucke, Yue Bai, Théo Hannotte, Mélanie Lavancier, Djamila Hourlier, Goedele Roos, Romain Peretti
to be submitted (2021).

[2] *A machine learning approach for the design of hyperbranched polymeric dispersing agents based on aliphatic polyesters for radiation curable inks*
Danny E. P. Vanpoucke, Marie A. F. Delgove, Jules Stouten, Jurrie Noordijk, Nils De Vos, Kamiel Matthyssen, Geert G. P. Deroover, Siamak Mehrkanoon, Katrien V. Bernaerts
submitted (2021).

[3] *Assigning probabilities to non-Lipschitz mechanical systems*
Danny E. P. Vanpoucke, and Sylvia Wenmackers
in revision (2020).

Editorial/Reviewing work

Guest Editor	Computational Nanoscience - How to Exploit Synergy Between Predictive Simulations and Experiment Curran Associates, Inc. (Jun 2010) series: Materials Research Society Symposium Proceedings Volume 1177 ISBN: 9781617383960
Review	A complete overview can be found at `https://publons.com/a/1216610/`.

- Diamond and Related Materials
- Journal of Superconducting Science and Technology
- Journal of Physics: Condensed Matter
- International Journal of Applied Ceramics Technology
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry
- Journal of Physical Chemistry
- Crystal Growth & Design
- Applied Physics Letters
- Materials Science in Semiconductor Processing
- Surface Science
- Frontiers in Physics
- Nanotechnology
- ACS Catalysis

Review Editor	Frontiers in Physics

List of Organized Workshops & Conferences

[1] *D-NL-HIT: Adhesives pilot-branch meeting 2020*
Maastricht University, The Netherlands, February 26^{th} 2020.

[2] *Condensed Matter Science in Porous Frameworks: On Zeolites, Metal- and Covalent-Organic Frameworks*
Groningen, The Netherlands, September 4 – 5^{th} 2016.

[3] *Spring School on Computational Tools for Materials Science*
Ghent University, April 13^{th} to April 17^{th} 2015.

List of Oral Presentations (as presenting author)

[1] *Ab initio diamond surfaces: functionalisation & dopant incorporation*
SBDD XXV, Cultureel Centrum Hasselt, Hasselt, Belgium, March 11-13th, 2020.

[2] *Tales of the odd duck in the pond*
Summer school sciencie communication, UAntwerpen, Antwerp, Belgium, July 2-3rd, 2019.**[Invited, Plenary]**

[3] *Ab initio investigation of Eu-doped diamond*
29th International Conference on Diamond and Carbon Materials, Valamar Lacroma Dubrovnik, Dubrovnik, Croatia, September 2-6th, 2018.

[4] *Adding Solids and Molecules: Metal-Organic Frameworks as Hybrid Materials*
27th International Materials Research Congress, Cancun, Mexico, August 19-24th, 2018.**[Invited]**

[5] *Luminescent Centres in Diamond: Ge & Eu Defect-Complexes*
27th International Materials Research Congress, Cancun, Mexico, August 19-24th, 2018.

[6] *Doping Diamond with Luminescent Centres: The Electronic Structure of Ge and Eu defect complexes*
General scientific meeting of the Belgian Physical Society 2018, Antwerp University, Antwerp, Belgium, April 11th, 2018.

[7] *Doping diamond with Ge and Eu: Understanding the electronic structure*
International Conference on Diamond and Carbon Materials 2017, Gothia Towers, Göteborg, Sweden, September 3-7th, 2017.

[8] *Spin dependent breathing flexible hybrid materials*
E-MRS spring meeting 2017, Palais de la musique et des congrès, Strasbourg, France, May 22-26th, 2017.

[9] *Understanding Breathing Metal-Organic Frameworks: Linking Theory to Experiment*
CMD26 Conference, Martiniplaza Conference Center, Groningen, The Netherlands, September 4-9th, 2016.

[10] *Metal-Organic Frameworks: When the whole is more than the sum of its parts*
General scientific meeting of the Belgian Physical Society 2016, Ghent University, Ghent, Belgium, May 18th, 2016.

[11] *Computational Solid State Physics and Chemistry.*
Virtual Winterschool on Computational Chemistry, February 3rd-9th, 2016. **[Invited]**

[12] *Computational Materials Science: where theory meets experiment*
39^{th} International Conference and exposition on Advanced Ceramics and Composites, Daytona Beach, Florida, United States, January 25-30^{th}, 2015. **[Invited]**

[13] *Doping of CeO_2 as a tunable buffer layer for coated superconductors: A DFT study of Mechanical and Electronic properties*
39^{th} International Conference and exposition on Advanced Ceramics and Composites, Daytona Beach, Florida, United States, January 25-30^{th}, 2015.

[14] *Tailoring metal-organic frameworks for adsorption applications.*
E-MRS Spring Meeting, Lille, France, May 26–30^{th}, 2014.

[15] *Calculating Hirshfeld-I charges in solids: implementation, pitfalls and applications*
Belgian Physical Society General Scientific Meeting 2013, Louvain-la-Neuve, Belgium, May 22^{nd}, 2013.

[16] *Investigation of tunable buffer layers for coated superconductors*
2013 meeting of the Belgian Ceramic Society, Diepenbeek, Belgium, April 19^{th}, 2013.

[17] *Atomic charges in solids: Calculating Hirshfeld-I charges for overlapping atoms from the electron density distribution*
ICAMM 2012 & VASP workshop, Nantes, France, June 11–16^{th}, 2012.

[18] *Tuning of CeO_2 buffer layers for coated superconductors through metal doping*
E-MRS 2011 Fall Meeting, Warsaw, Poland, September 19–23^{rd}, 2011.

[19] *Pt nanowires on Ge(001): Sheep in Wolf's Clothing?*
(First prize at the "2011 Young Speaker Contest")
Belgian Physical Society General Scientific Meeting 2011, Namur, Belgium, May 25^{th}, 2011.

[20] *DFT study of $La_2Ce_2O_7$: a Question of Order*
2011 meeting of the Belgian Ceramic Society, Mons, Belgium, February 7^{th}, 2011.

[21] *The formation of self-assembled nanowire arrays on Ge(001): a DFT study of platinum induced nanowires*
MRS Spring meeting, San Fransisco, USA, April 13–17^{th}, 2009.

[22] *DFT Study of Pt Induced Nanowires*
DPG Spring meeting, Dresden, Germany, March 22–27^{th}, 2009.

[23] *Nanowires on the Germanium-Platinum(001)-surface*
CW-study group Spectroscopy and Theory, Luntheren, The Netherlands, January 28–29^{th}, 2008.

List of Poster Presentations (as presenting author)

[1] *Materials design through ensemble learning: The impact of very small data sets*
ACOS Symposium 2020: "Machine Learning from Big Data to Multi-scale modeling", online, Oktober 28^{th}, 2020.

[2] *Machine Learning based design with small data sets*
RSC Chemical Science Conference 2020, online, September 29-30^{th}, 2020.

[3] *Ab initio Diamond surfaces: functionalisation and dopant incorporation*
SBDD XXV, Cultureel Centrum Hasselt, Hasselt, Belgium, March 11-13^{th}, 2020.

[4] *Calculating Vibrational spectra in solids: From fingerprinting defects in diamond to the impact of water in molecular crystals.*
VSC userday 2019, Paleis der Academiën, Brussels, Belgium, June 4^{th}, 2019.

[5] *First principles calculation of vibrational spectra in solids: From fingerprinting defects in diamond to the impact of water in molecular crystals.*
Belgian Physical Society Meeting, ULB, Belgium, May 22^{nd}, 2019.

[6] *Doping Diamond with Luminescent Centres: The Electronic Structure of Ge and Eu defect complexes*
VSC userday 2018, Paleis der Academiën, Brussels, Belgium, May 22^{nd}, 2018.

[7] *Doping Diamond with Luminescent Centres: The Electronic Structure of Ge and Eu defect complexes*
SBDD XXIII, Cultureel Centrum Hasselt, Hasselt, Belgium, March 7-9^{th}, 2018.

[8] *Revisiting the neutral C-vacancy in diamond: Localization of electrons in DFT*
QCB13: Quantum Chemistry in Belgium, Universite Libre de Bruxelles, Brussels, Belgium, January 30^{th}, 2018.

[9] *Tuning the electronic structure in Metal-Organic Frameworks: When molecules and metal oxides come together*
Summer school: Upscaling techniques for mathematical models involving multiple scales, Hasselt University, Hasselt, Belgium, June 26-29^{th}, 2017.

[10] *HPC-based materials research: From Metal-Organic Frameworks to Diamond*
VSC userday 2017, Paleis der Academiën, Brussels, Belgium, June 2^{nd}, 2017.

[11] *Revisiting the neutral C-vacancy in diamond: Localization of electrons in DFT*
E-MRS Spring Meeting 2017, Palais de la musique et des congrès, Strasbourg, France, May 22-26^{th}, 2017.

[12] *Tuning the electronic structure in Metal-Organic Frameworks: When molecules and metal oxides come together*
E-MRS Spring Meeting 2017, Palais de la musique et des congrès, Strasbourg, France, May 22-26^{th}, 2017.

[13] *Revisiting the neutral C-vacancy in diamond: Localization of electrons in DFT*
SBDD XXII, Cultureel Centrum Hasselt, Hasselt, Belgium, March 8-10^{th}, 2017.

[14] *Breathing Metal-Organic Frameworks: From spin-dependent breathing to electronic structure tuning*
tUL Life Science Research Day 2016, Alden Biesen, Bilzen, Belgium, October 5^{th}, 2016.

[15] *Understanding Experiments: the Power of First Principle Simulations of Metal-Organic Frameworks*
Quantum Chemistry In Belgium 12, KULeuven, Kasteelpark Arenberg 41, 3001 Heverlee, Belgium, February 16^{th}, 2016.

[16] *Understanding Experiments: the Power of First Principle Simulations of Metal-Organic Frameworks*
Annual Scientific Meeting IAP P7/05, Hasselt, Belgium, September 11^{th}, 2015.

[17] *Low dimensional physics in Metal-Organic Frameworks: a DFT study of breathing MIL-47*
Belgian Physical Society Meeting, Liège, Belgium, May 13^{th}, 2015.

[18] *Quasi-1D Physics in Breathing Metal-Organic Frameworks*
Meeting of the Dutch Zeolite Association On hybrids and Zeolites, Ghent, Belgium, October 7^{th}, 2014.

[19] *New Quasi-1D Materials: DFT study of Breathing Metal Organic Frameworks.*
Annual Scientific Meeting IAP P7/05, Louvain-La-Neuve, Belgium, September 19^{th}, 2014.

[20] *Hirshfeld-I charges: from Molecules to Solids. Implementation, pitfalls and applications*
Quantum Chemistry in Belgium, eleventh edition, Namur, Belgium, January 23^{rd}, 2014.

[21] *Functionalized Metal-Organic Frameworks: MIL-47(V)+X a computational investigation of its properties*
IAP7 meeting, Ghent University, September 18^{th}, 2013.

[22] *Calculating Hirshfeld-I charges in solids: implementation, pitfalls and applications*
DFT2013, Durham, UK, September 9–13^{th}, 2013.

[23] *Chemistry in Solids; Extending the Hirshfeld-I method.*
Quantum Chemistry in Belgium, tenth edition, Etterbeek, Belgium, February 10^{th}, 2012.

[24] *Tuning of CeO_2 buffer layers through doping*
Seventh International Conference on Inorganic Materials, Biarritz, France, September 12–14^{th}, 2010.

[25] *CO Adsorption on Pt induced Nanowires*
Mesa$^+$-day, Enschede, The Netherlands, September 21^{st}, 2009.

[26] *Road To Nanotechnology*
Science as Art competition at the MRS Spring meeting, San Fransisco, USA, April 13–17^{th}, 2009.

[27] *Formation of Pt Induced Nanowires on Ge(001): a DFT study*
CW-study group Spectroscopy and Theory, Luntheren, The Netherlands, January 26–27^{th}, 2009.

[28] *The Germanium-Platinum(001) surface as a template for nanowires*
ICTP 14^{th} international workshop on computational physics and material science: Total energy and force methods, Trieste, Italy, January 8–10^{th}, 2009.

[29] *The Germanium-Platinum(001) surface as a template for nanowires*
CECAM Workshop: Structural, electronic and transport properties of quantum wires, Lyon, France, June 9–12^{th}, 2008.

[30] *The Germanium-Platinum(001) surface as a template for nanowires*
FOM Physics@Veldhoven, Veldhoven, the Netherlands, January 22–23^{rd}, 2008.

[31] *Depositing Pt on Ge(001): Where do the Pt Atoms Go?*
Mesa$^+$-day, Enschede, The Netherlands, September 11^{th}, 2007.

[32] *Depositing Pt on Ge(001): Where do the Pt Atoms Go?*
CW-study group Spectroscopy and Theory, Luntheren, The Netherlands, January 29–30^{th}, 2007.

[33] *Depositing Pt on Ge(001): Where do the Pt Atoms Go?*
FOM Physics@Veldhoven, Veldhoven, the Netherlands, January 23-24^{th}, 2007.

[34] *Surface and Interface calculations: GaAs/Ge, $LaAlO_3/SrTiO_3$ and Pt on Ge(001)*
NIC winterschool 2006: Computational Nanoscience: Do It Yourself!, Forschungszentrum Jülich, Germany, February 14–22^{nd}, 2006.

International Schools and Conferences

[1] *Workshop Machine Learning and Coatings technology*
Hochschule Niederrhein, Krefeld, Germany, September 2^{nd}-6^{th}, 2019.

[2] *Research visit Westfälische Hochschule*
Group of Prof. dr. Klaus-Uwe Koch, Recklinghausen, Germany, July 29^{th} - Augustus 2^{nd}, 2019.

[3] *Summer school on data science*
Data science and Knowledge Engineering, Maastricht University, Maastricht, The Netherlands, June 26-28^{th}, 2019.

[4] *SBDD XXIV (Hasselt Diamond Workshop 2019)*
Cultuur Centrum Hasselt, Hasselt, Belgium, March 13-15^{th}, 2019.

[5] *Summer school: "Upscaling techniques for mathematical models involving multiple scales"*
Hasselt University, Hasselt, Belgium, June 26-29^{th}, 2017.

[6] *SBDD XXI (Hasselt Diamond Workshop 2016)*
Cultuur Centrum Hasselt, Hasselt, Belgium, March 9-11^{th}, 2016.

[7] *CECAM Workshop: "Basic techniques and tools for development and maintenance of atomic scale software"*
CECAM-HQ-EPFL, Lausanne, Switzerland, October 13-17^{th}, 2014.

[8] *Challenges towards Exascale Computing*
Ghent University, Ghent, Belgium, May 16^{th}, 2011.

[9] *Frontiers of Density Functional Theory: A One Day Symposium in Honor of Weitao Yang*
Academy Palace of the Royal Flemisch Academy of Belgium for Science and the Arts, Brussels, Belgium, November 15^{th}, 2010.

[10] *QCB9 (Quantum Chemistry in Belgium)*
Louvain-La-Neuve, Belgium, January 26^{th}, 2010.

[11] *Symposium on Carbon Nanostructures*
University of Antwerp, Antwerp, Belgium, September 15^{th}, 2008.

[12] *Workshop: Fundamentals of Nanotechnology*
Mesa^{+}, Enschede, The Netherlands, November 5–9^{th}, 2007.

[13] *NIC winterschool 2006: Computational Nanoscience: Do It Yourself!*
NIC, Forschungszentrum Jülich, Germany, February 14–22^{nd}, 2006.

[14] *Ψ_k 2005 Conference: Toward atomistic materials design*
psi-k and ESF, Schwäbisch Gmünd, Germany, September 17–22^{nd}, 2005.