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

Current Affiliation:

Universiteit Hasselt - Hasselt University
Wide Bandgap Materials (WBGM)
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Work Experience

2016– : **FWO Postdoctoral Fellow**
Hasselt University

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

2014–2016: **FWO postdoctoral Fellow**
Ghent University

In the Center for Molecular Modeling (CMM) of Prof. Dr. Ir. V. Van Speybroeck, at the 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 the 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: **PhD/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

- 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

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”*

2015 Granted 1.1 million hours CPU time on the Flemish Tier-1 supercomputer, for the project:*“The electronic structure of functionalized luminescent Metal-Organic Frameworks”*

2014 Granted 1.8 million hours CPU time on the Flemish Tier-1 supercomputer, for the project:*“The electronic and magnetic structure of Breathing Metal-Organic Frameworks”*

2013 Granted 3.2 million hours CPU time on the Flemish Tier-1 supercomputer, 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

Fortran95, Fortran2003, Delphi, Pascal, Java, C++(basics)

bash script, HTML, CSS, Java script

LaTeX 2_ε, MS Office, xmgrace, Maple, gnuplot, Jasc Paint Shop

Professional Membership

Belgian Physical Society (BPS)

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] *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)

[2] *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)

[3] *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)

[4] *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)

[5] *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. $\mathbf{55}(\mathbf{3})$, 564-571 (2015)

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

[7] *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. $\mathbf{5}$, 1738–1748 (2014).

[8] *Aliovalent Doping of CeO2: 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 $\mathbf{2}$, 13723–13737 (2014).

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

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

[11] *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. $\mathbf{97}(\mathbf{1})$, 258-266 (2014)

[12] *New Functionalized Metal-Organic Frameworks MIL-47-X (X = -Cl, -Br, -CH_3, -CF_3, -OH, -OCH_3): Synthesis, Characterization and CO2 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 $\mathbf{117}(\mathbf{44})$, 22784-22796 (2013)

[13] *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).

[14] *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).

[15] *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).

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

[17] *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).

[18] *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).

[19] *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).

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

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

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

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

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

[5] *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.

[6] *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] *The role of atomic models in AIM partitioning schemes*
Danny E. P. Vanpoucke, Sofie Van Damme, and Patrick Bultinck
In preparation

[2] *Assembly of a variety of mono-, tetra- and dodecanuclear copper(II) complexes and copper(II) coordination polymers from aminopolyalcohols and amine polyacids in aqueous solution: structural and magnetic characterization*
Petra Lommens, Kristof Van Hecke, Adam K. Budniak, Arnaud Hillion, Sofie Van Damme, Danny E. P. Vanpoucke, Margriet J. Van Bael, Isabel Van Driessche
Dalton Trans.(submitted)

[3] *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. (accepted) doi: 10.1021/acs.inorgchem.5b02805 (2016)

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

List of Oral Presentations

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

[2] *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]**

[3] *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

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

[5] *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

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

[7] *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.

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

[9] *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.

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

[11] *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.

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

[13] *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

[1] *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

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

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

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

[5] *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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[20] *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 14–22nd, 2006

International Schools and Conferences

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

[2] *Challenges towards Exascale Computing*
Ghent University, Ghent, Belgium, May 16th, 2011

[3] *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 15th, 2010

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

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

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

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

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