

Curriculum Vitae Nele Moelans

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Personalialia

<http://nele.studentenweb.org>
<https://www.mtm.kuleuven.be/Onderzoek/Semper/SolMicS>
https://www.researchgate.net/profile/Nele_Moelans
<https://www.linkedin.com/in/nele-moelans-57b1731>

Name: Nele Moelans
Date of birth: July 12, 1977
Place of Birth: Leuven
Nationality: Belgian

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Job experience and education

- October 2015 - : **Associate professor** at KU Leuven (BOF-KU Leuven Research professor), Department of Materials Engineering
 - **Research expertise and interests:** phase-field modelling of microstructure evolution, calculation of multi-component phase diagrams (CALPHAD), equilibrium and non-equilibrium thermodynamics, diffusion (couple) experiments and modeling, phase transformations, interfaces, grain growth, lead-free soldering, thermodynamics and kinetic modeling of nanowire growth, HEA (or multi-principle alloys), materials informatics, ICME
 - **Teaching:**

- * Computational Thermodynamics in Materials Design, master in Materials Science, KU Leuven (B-KUL-H02V3A)
- * Materials Modeling and Simulation Techniques, Master in Materials Science, KU Leuven (H0S49A)
- * Structuurgeneese van materialen (Structure formation of materials), Bachelor in Materials Science, KU Leuven (B-KUL-H01I8A)
- * Athens course at KU Leuven on "Small Scale Modeling Techniques for Materials" (Nov. 2015, Nov. 2016)
- October 2010 - September 2015: **Assistant professor** at KU Leuven (BOF-KU Leuven Research professor), Department of Materials Engineering.
- October 2006 - September 2010: **Postdoctoral Fellow of the Research Foundation - Flanders (FWO-Vlaanderen)** at Department of Materials Engineering, KU Leuven, Belgium
- September 2008 - August 2009: **Postdoc at Lawrence Livermore National Laboratory (LLNL)**, Condensed Matter & Materials Division, California, USA.
- October 2002 - September 2006: **Doctoral student in Engineering granted by the Institute for the Promotion of Innovation by Science and Technology in Flanders (IWT-Flanders)** affiliated with Department of Materials Engineering, KU Leuven
 - Doctorate obtained on May 19, 2006 with *Summa cum laude with the congratulations of the Examination Board* (only awarded in exceptional circumstances, at most 5% of the doctorates in engineering at KU Leuven)
 - Topic: Phase-field simulations of grain growth in materials containing second-phase particles; Abstract and thesis text: <http://hdl.handle.net/1979/309>
- September 1997 - June 2002: **Master of Science in Materials Engineering** at Department of Materials Engineering, KU Leuven
 - M.S. degree with *Summa cum laude*
 - Master thesis: Calculation of phase diagrams for lead-free solder alloys based on Bi-In-Sn-Zn; Abstract (English and Dutch) and thesis text (Dutch only) on <http://nele.studentenweb.org/docs/thesis.pdf>
- Summer 2001: **Summer training at R&D Umicore**, Olen, Belgium
 - Topic: Ex-situ pO_2 -measurements of non-ferrous slags
- Summer 2000: **Summer training at IMEC (Interuniversity MicroElectronics Center)**, Leuven, Belgium
 - Topic: MOKE (Magneto Optical Kerr Effect) - measurements of soft magnetic materials
- 1996 - 1997: Preparatory year on mathematics, KU Leuven
- 1995 - 1996: Higher education for dance and dance pedagogy (Hoger Instituut voor Dans en Danspedagogie), Lier, Antwerp, Belgium
- 1989 - 1995: High school, Paridaens Instituut, Leuven, Option Greek-Latin

Memberships, commissions, responsibilities

- Member (2000-2003) and secretary (2003-2006) of the P.O.C.-commission for Materials Engineering at KU Leuven
- Member of COST 531 Lead-free solder materials and COST 535 Thermodynamics of alloyed aluminides (2005-2007)
- Management Committee member and working group leader in COST MP0602 (2007 - 2011)
- Spokes person KU Leuven in the SRN (Scientific Research Network) on Computational modeling for materials (sponsored by FWO-Flanders) (2010 - 2014 and 2014-2018)
- Examiner PhDs at and outside KU Leuven
- Guest editor of 2 special issues of an international journal on multi-scale modeling
 - "Multi-Scale Modeling of Moving Interfaces in Materials". Mathematics and Computers in Simulation (Elsevier), 80 (7), 1359-1360, March 2010.
 - "Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models". Computational Material Science (Elsevier), Vol 66, January 2013.
- Member high performance computing steering committee, KU Leuven (since 2014)
- Member User Committee Flemish Supercomputer Centre (VSC) (2014-2017)
- Reviewer national and international project proposals (KU Leuven, SNSF, NSERC, NCN-Poland, ...)
- Evaluator professor candidates
- Reviewer journal papers for various journals in the field of materials science, alloy development and characterization and computational materials science (such as Acta Mater., Comp. Mater. Sci, Phys. Rev. B/E/Lett., MSMSE, CALPHAD, Scripta Mater., Scientific reports ...)

Publication record

- Unique research identifier (ORCID): orcid.org/0000-0003-3361-2954
- Google scholar: https://scholar.google.be/citations?hl=nl&user=x_x0MmQAAAAJ
- >50 publications in internationally reviewed journals
- 4 contributions in books
- >20 conference proceedings
- >80 conference presentations of which 25 invited
- h-index: 14 (Scopus); 15 (Googlescholar)
- Total citations: >1000 in Scopus; >1400 in Googlescholar

Grants and honors

Besides the doctoral grant of IWT-Flanders, two 3-year postdoctoral fellowships of FWO-Flanders and a 10-year BOF-KU Leuven research professorship as specified in the section Education and Job Experience,

- PhD degree obtained with *Summa cum laude with the congratulations of the Examination Board* (only awarded in exceptional circumstances, at most 5% of the doctorates in engineering at KULeuven)
- Ph. D. frontier research poster award at the Gordon Research Conference on High Temperature Materials, Processes and diagnostics, Colby College, Waterville, ME, July 16-21 2006: "3D Phase field simulations of grain growth in thin films: pinning effect of second-phase particles and thermal grooving"
- Most downloaded and *highly cited* paper of CALPHAD – Computer Coupling of Phase Diagrams and Thermochemistry: "An introduction to phase-field modeling of microstructure evolution"
- Highlight lecture at Euromat 2009, Glasgow, UK: "Phase field simulations of recrystallization in Al-Mn alloys containing Al₆Mn precipitates"
- STT grant (Foundation for applied Thermodynamics, KTH, Sweden) to attend the Winter School on Fundamentals of Thermodynamic Modeling of Materials, Saclay, France, Nov 15-19, 2010.
- Research paper in top 10 of most downloaded papers in April to June 2011 of CALPHAD – Computer Coupling of Phase Diagrams and Thermochemistry: "Calculation of phase equilibria for an alloy nanoparticle in contact with a solid nanowire"
- Discussion leader, Gordon Research Conference Physical Metallurgy: Evolution of Metals Structures: Modeling, Characterization and Design. Stonehill College, Easton, MA, USA, July 31- Aug 5, 2011.
- CALPHAD poster award. Best poster presented at CALPHAD XLII Conference, San Sebastian, Spain, 2013: "New Quantitative Phase-Field Model for Elastically Inhomogeneous Systems" (300 USD)
- ERC Starting Grant 2016 "Unravelling interdiffusion effects at material interfaces – Learning from tensors of microstructure evolution simulations (INTERDIFFUSION)" (1.5 Meuro EUR)
- Acta Materialia Outstanding Reviewer in 2016 (200 \$).
(<https://www.journals.elsevier.com/acta-materialia/news/acta-journals-outstanding-reviewers-in-2016-acta-materialia>)
- Marie Skłodowska-Curie Actions Seal of Excellence (25 April 2017). Project title: An innovative multi-scaled model on the microstructure evolution and deformation of high entropy alloys. Researcher: Hong Liu. Supervisor: Nele Moelans.

Organization conferences, workshops, seminars

- Organizer of the symposium Towards Realistic Three-Dimensional Phase-Field Simulations for the Evolution of Polycrystalline Structures on the SIAM - conference on Mathematical Aspects of Materials Science, Philadelphia, May 2008
- Organizer of the workshop Multi-Scale Modeling of Moving Interfaces in Materials, 2-4 July, 2008, K.U. Leuven, Belgium, with G. Samaey
 - Sponsors: Res Metallica (Arcelor Mittal, Bekaert and Umicore) – SRN Surface modification of materials – SRN Advanced numerical methods for mathematical models – SRN Structural and chemical characterization of materials at the micro- and nanoscale;
- Member scientific committee of Second Decennial Symposium on Phase-Field Modelling in Materials Science, Aachen, September 2009 (chairmen I. Steinbach and L.-Q. Chen)
- Member international advisory board of TOFA 2010, Discussion Meeting on Thermodynamics OF Alloys, Porto, Portugal, 12-17 September 2010
- Organizer COST MP0602 Working Group 3 meeting on Study of the Interfacial Reactions in Lead-Free Solder Joints for High Temperature Applications, K.U. Leuven, Belgium, January 6-7, 2010.
- Organizer of the workshop Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, 12-14 January, 2011, K.U. Leuven, Belgium, together with G. Samaey
 - Sponsors: Res Metallica (Arcelor Mittal, Bekaert and Umicore) – SRN Surface modification of materials – SRN Advanced numerical methods for mathematical models – SRN Structural and chemical characterization of materials at the micro- and nanoscale – SRN Computational modeling for materials; COST MP0602 Advanced Solder Materials for High Temperature Application (HISOLD) – their nature, design, process and control in a multiscale domain; FWO-Flanders
- Co-organiser symposium on Thermodynamics and kinetics: modelling of phase diagrams and microstructure evolution (D34) Euromat 2011, Montpellier, France, 12-15 September (Organiser: Hans Seifert, Co-organisers: Rainer Schmid-Fetzer, Nele Moelans)
- Workshop on Mesoscale and continuum scale modeling of materials defects, Nov. 13-16 2012. Organizers: V. Shenoy, N. Ghoniem, David Kinderlehrer, Nele Moelans, John Lowengrub. Part of a series of workshops on modeling of defects in materials organized at IPAM, Institute for Pure and Applied Mathematics, UCLA, California, USA.
- Local organisation of Computational Thermodynamics and Kinetics Seminar (ThermoCalc user meeting), Leuven, April 23-24, 2013.
- Member scientific committee of the Third International Symposium on Phase Field Method –PFM 2014, State College, Pennsylvania, August 26-29, 2014 (organised by I. Steinbach and L.-Q. Chen)
- Res Metallica 2016, Looking deep into materials, KU Leuven, Leuven, Belgium, May 11, 2016.

- Co-organiser symposium Microstructure Evolution in Materials: Mechanisms, Properties, Manufacture at Multiscale Materials Modelling (MMM), Oct 9-14, 2016, Dijon, France.
- Res Metallica 2017, Multi-scale modeling of materials, KU Leuven, Leuven, Belgium, May 17, 2017.
- Co-organiser session on Multiscale modelling of microstructure evolution and materials mechanics at IWCMM, Belgium (Leuven), 20-22 September 2017.
- Co-organiser symposium Advanced modelling techniques: phase field and diffuse interface approaches at 16th European Mechanics of Materials Conference, EMMC16, March 16-18, 2018, Nantes (France).

PhD students

Completed

- L. Vanherpe (M.S. degree in Computer Science, K.U.Leuven), Acceleration strategies for phase field simulation of grain growth in polycrystalline materials, October 2005 - September 2010, promotors: S. Vandewalle, B. Blanpain(, financed by the IUAP-program DISCO)., Defense September 2010.
- J. Heulens (M.S. degree in Materials Engineering, K.U.Leuven), Isothermal crystallization of metallurgical slags: Phase field simulations combined with in situ experiments, October 2007 - December 2011, promotors: N. Moelans, B. Blanpain, granted by IWT-Vlaanderen.
- Y. Eichhammer (M.S. degree in Engineering from Ecole Centrale de Lille), Thermodynamic and Kinetic Description of Nanowires and Nanowire growth, promotoren: N. Moelans and M. Heyns, November 2007 - February 2012, IMEC funding for fundamental doctoral research.
- V. Yadav (M.S. degree in Metallurgy and Materials Engineering from Indian Institute of Technology Bombay, IIT Bombay), Modeling and simulation of grain growth and coarsening in polycrystalline materials, started in February 2009, promotors: P. Wollants, N. Moelans. Financed by G.0362.09N (FWO funding).
- A. Durga (B.S. degree in Metallurgy and Materials Engineering, Indian Institute of Technology Madras, IIT Madras), Development of an elastoplastic phase-field model for multi-phase systems, October 2010 - March 2015, promotors: N. Moelans and P. Wollants, financed by OT/07/040 and CREA/12/012 (KU Leuven funding).
- H. Ravash (M.S. degree in Materials Science from Chalmers University, Sweden), 3D phase-field simulations of sintering and coarsening in polycrystalline multi-phase materials, September 2010 - December 2014, promotors: N. Moelans, J. Vleugels. Financed by SIM project SOPPOM, SBO absCIGS.
- Yuanyuan Guan (M.S. degree in Materials Engineering, KU Leuven), Development of a method to determine the solubility ranges of intermetallic compounds in metal-metal connections, September 2011 - November 2015, Promotor: N. Moelans, financed by OT/07/040 and CREA/12/012 (KU Leuven funding).

- Evelien De Wilde (M.S. degree in Chemistry, U Ghent), Methodology Development and Experimental Determination of the Origin of Sticking Copper Droplets in Pyrometallurgical Slags, September 2011 - December 2015. Promotors: Kim Verbeken (Ughent), N. Moelans. Financed by IWT-Baekeland with industrial promotor Umicore.
- Jingjing Liu (M.S. degree Materials Science and Engineering, Zhejiang University, China), In-situ observation and phase-field simulation of crystallization and dissolution phenomena in CaO-Al₂O₃-SiO₂ slags, October 2011 -August 2016. Promotors: N. Moelans and M. Guo. Financed by a CSC grant (China Scholarship Council).
- Andrea Isabel Gil Santos (M.S degree in material physics from Complutense University of Madrid (UCM); Master in Laser Technology at Polytechnic University of Madrid (UPM)), Phase diagram assessment and alloy characterization of ternary Mg rich Mg-Si-Ca and Mg-Si-Sr alloys for biomedical applications, Sept 2012 - May 2017, Promotors: O. Vanderbiest, N. Moelans. Financed by the Marie Curie International training network MagnIM.
- Inge Bellemans (M.S. degree in Engineering Science, Materials, U Ghent), Metal droplet entrainment by solid particles in slags: A combined phase field – experimental approach, Oct 2013-May 2017. Promotors : Kim Verbeken (U Ghent), Nele Moelans. Financed by FWO PhD fellowship.

Ongoing

- Nabi Nabioli (M.S degree in Microtechnology and nanoscience Chalmers University of Technology, Gothenburg, Sweden), Processing induced changes of mechanical stresses in and near Cu Through Silicon Vias (TSVs): a finite element modelling study, December 2011 (end foreseen for end 2016), Promotors: I. Dewolf, N. Moelans. Financed by Imec, Leuven.
- Athina Puype (M.S. degree in Engineering Science, Materials, U Ghent), Development of improved ferritic/martensitic creep-resistant steels for nuclear energy, start Sept 1, 2014. Promotors : Jilts Sietsma, Nele Moelans, financed by OCAS+SCK-CEN.
- Lin Hou (M.S. degree in Materials Engineering, KU Leuven), Miniaturization of Solder Balls for 3D Silicon Chip Interconnection, start October 1, 2015. Promotors: I. Dewolf, N. Moelans. Financed at Imec, Leuven.
- Yuri Coutinho (B.S. degree Mechanical Engineering Rio de Janeiro State University, M.S. degree Materials Science and Engineering, Alfred University), Phase-field modeling and quantification of microstructure evolution at multi-component material joints, start May 1, 2017. Promoters: N. Moelans, L. Delathauwer, financed by ERC-StG-2016 INTERDIFFUSION (n° 714754).
- Sourav Chatterjee (M.S. Materials Science IIT Bombay), Phase-field modeling of microstructure evolution in mechanically loaded material joints, start Aug 1, 2017. Promoters: N. Moelans, financed by ERC-StG-2016 INTERDIFFUSION (n° 714754).

Postdocs

- Hong Liu, PhD from Monash University in 2015. FWO Pegasus Marie Curie fellowship March 2017-Febr 2020. Research project: Phase-field modeling and simulation of twinning in materials with hexagonal symmetry.
- Hou Yanhui, Wuhan University of Technology, China. March - May 2011 funded by National Natural Science Foundation of China, October 2011 - March 2012, funded by EXPERTS Scholarship (Erasmus Mundus, Europe). Research topic: ab initio calculations of surface and interfacial properties of precipitates in Al-Cu-Mg-(Ag) alloys.
- Yuan Yuan (PhD in 2012 at Central South University, China). Research project: Integrated approach for predicting the microstructure evolution of multi-component joints based on combinatorial key-experiments, phase diagram calculation and microstructure simulation. Financed as FWO Pegasus Marie Curie postdoctoral fellow, Oct 2012 - Sept 2016.
- Kunok Chang (PhD in 2011 at Penn. State University, USA). Research topic: Phase-field simulations of grain growth and the effect of texture and pinning precipitates on grain growth. Oct 2012-Aug 2013. Financed from CREA/12/012 (KU Leuven funding).
- Liesbeth Vanherpe (PhD in 2010 at KU Leuven, Department of Computer Science). Research topic: Bounding box sparse data structure framework for phase field simulations of grain growth in polycrystalline materials. Sept-Oct 2010. Financed from OT/07/040 (KU Leuven funding).