

Prof. Noël Jakse

Address

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Curriculum Vitae

Education:

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|-------------|---|
| 13.05.1966 | born in Saint-Avold, France |
| 1986 – 1989 | Bachelor in Physics
University of Lorraine, Metz, France |
| 1989 – 1991 | Master in Physics and Material Science
University of Lorraine, Metz, France |
| 1991 – 1993 | Ph.D. thesis in Physics and Mechanical Engineering
<i>Title Contribution to the study of structure and thermodynamics
of liquid metals by the integral equations theory</i>
University of Lorraine, Metz, France
(Advisors: Prof. J-L.. Bretonnet) |
| 1993 – 1998 | Habilitation in Physics, University of Lorraine, Metz |

Professional experience:

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| 1992 – 1994 | Junior Lecturer in Physics and Material Science
University of Lorraine, Metz, France |
| 1994 – 2006 | Senior Lecturer in Physics and Material Science
University of Lorraine, Metz, France |
| 2006 – present | Full Professor in Physics and Chemistry of solids
University Grenoble Alps
Grenoble Institute of technology (Grenoble-INP), Grenoble, France |

Awards and functions

- 2006 – Present Reviewer for ANR, DFG, NUS Syngapour
- 2009 – 2012 Director of International Relation and student exchange of PHELMA School
UGA-Grenoble-INP, Grenoble France
- 2013 – 2019 Head of Thermodynamic, modelling and optimization of processes (TOP) research group
SIMAP Laboratory, UGA-Grenoble-INP, Grenoble France
- 2011 – present Editorial Board Member of Scientific Reports (Nature)
- 2018 – 2021 Member of the Scientific Board, GDR ModMat (Modelling on Materials)
- 2019 – Present International Scientific Board Member
Liquid and Amorphous Metals (LAM) international Conference
- 2019 Member of the Organizing committee
Liquid and Amorphous Metals International Conference (LAM17), Lyon, France
- 2019 Member of the Organizing committee
Diffusion in Solid and Liquid (DSL) international Conference
- 2019 – present Member of the chairs Machine learning for mAterial desiGN
and Efficient sysTems (MAGNET)
- 2019 – Present Member of the Scientific Board, Industry 4.0 division
Multidisciplinary Institute of Artificial Intelligence (MIAI)
<https://miai.univ-grenoble-alpes.fr/>, University Grenoble Alps, Grenoble, France
- 2020 – present Editorial Board Member of Metals (MDPI)
- 2021 – Present Member of the Scientific Board
Common research Laboratory: SIMAP and C-TEC Constellium, Grenoble France
- 2022 – present Member of the Scientific Committee of DIADEM
DIScovery Acceleration for the Deployment of Emerging Materials,
National Exploratory Research Program (2022 – 2029)

Areas of research

- Statistical physics, Condensed matter and materials science, especially disordered states of matter
- Computer simulation at the atomic scale and related machine learning tools
- Density function theory
- Relation between Structure and dynamics as well as thermodynamics of liquids, amorphous metals, and oxides
- Solidification mechanisms and nucleation phenomena in metallic melts
- Dynamic heterogeneity in glass forming materials
- Structure and dynamics metallic melts under high pressure

Ten selected publications

- [1] S. Becker, E. Devijver, R. Molinier and **N. Jakse**,
Unsupervised topological learning approach of crystal nucleation in pure Tantalum,
Machine Learning and the Physical Sciences Workshop at the 35th Conference on Neural Information Processing Systems (NeurIPS 2021)
- [2] F Demmel, L Henet, **N Jakse**,
The intimate relationship between structural relaxation and the energy landscape of monatomic liquid metals,
Scientific Reports **11**, 11815 (2021).
- [3] S. Becker, E. Devijver, R. Molinier, **N. Jakse**,
Glass-forming ability of elemental zirconium
Physical Review B **102**, 104205 (2020).
- [4] E. Sondermann, **N. Jakse**, K. Binder, A. Mielke, D. Heuskin, F. Kargl, and A. Meyer,
Concentration dependence of interdiffusion in aluminum-rich Al-Cu melts,
Phys. Rev. B, **99**, 024204 (2019).
- [5] A Pasturel, **N Jakse**,
Effect of pentagonal-coordinated surface on crystal nucleation of an undercooled melt,
Scientific Reports **8**, 14314 (2018).
- [6] A. Pasturel, **N. Jakse**,
Atomic-scale structural signature of dynamic heterogeneities in metallic liquids,
npj Computational Materials **3** , 33 (2017).
- [7] K. N. Lad, **N. Jakse**, A. Pasturel,
Signatures of fragile-to-strong transition in a binary metallic glass-forming liquid,
The Journal of Chemical Physics **136**, 104509 (2012).
- [8] **N Jakse**, A Pasturel,
Glass forming ability and short-range order in a binary bulk metallic glass by ab initio molecular dynamics,
Applied Physics Letters **93**, 113104 (2008).
- [9] **N. Jakse**, A. Pasturel,
Liquid-liquid phase transformation in silicon: evidence from first-principles molecular dynamics simulations,
Physical Review Letters **99**, 205702 (2007).
- [10] **N Jakse**, A Pasturel,
Local order of liquid and supercooled zirconium by ab initio molecular dynamics,
Physical Review Letters **91**, 195501 (2003).