DR. ACHRAF ATILA

E-mail: achraf.atila@uni-saarlande.de
E-mail: achraf.atila@gmail.com

Universität des Saarlandes,
Lehrstuhl für Materialsimulation,
Campus C 6.3, Saarbrücken D-66123

EDUCATION

PhD Friedrich-Alexander-University of Erlangen-Nürnberg, (2018-2023)
Thesis: Influence of the structure and topology on the deformation behavior and fracture of oxide glasses."
Advisor: Prof. Dr.-Ing. Erik Bitzek
Grade: Very good

M2 **University of Hassan II**, Physics of Materials and Nanomaterials, 2017
Thesis: "Molecular dynamics simulation of the thermodynamic and structural properties of calcium aluminosilicate glasses."
Advisors: Prof. Said Ouaskit and Prof. Abdellatif Hasnaoui

M1 **University of Hassan II**, Physics and New Technologies, 2016

BS **University of Hassan II**, Physics and Applications, 2015

RESEARCH EXPERIENCE

Postdoctoral Research Associate, Universität des Saarlandes (01.07.2022 –)

Guest Scientist, Max-Planck-Institut für Eisenforschung (MPIE) (01.07.2021 – 31.12.2022)

Research Associate, Friedrich-Alexander-University of Erlangen-Nürnberg (16.04.2018 – 15.04.2022)

Research Internship, Faculty of Sciences Ben M'SIK – (LPMC), CASABLANCA, (01.02.2017 – 15.07.2017)
Advisor: Prof. Said Ouaskit, Prof. Abdellatif Hasnaoui

PROJECTS AND GRANTS

CPUH project (Co-PI): Submitted proposal to Jülich supercomputing center to the atomic scale processes of friction,
Granting period: 01.11.2023 – 31.10.2024,
Total CPUH: 13 Million core hours
CPUH project: Granted computing proposal at Jülich supercomputing center to study the deformation and failure mechanisms of bulk metallic glasses,
Granting period: 01.11.2022 – 31.10.2023,
Total CPUH: 29 Million core hours

TEACHING EXPERIENCE

Teaching, Universität des Saarlandes (01.07.2023 –)

- Oct.2023-Feb. 2024, Computer Simulations in Materials Physics, (Supervised 2 students projects) (~30 h)

Teaching Assistance, Universität des Saarlandes (01.07.2022 –)

- Oct.2022-Feb. 2023, Computer simulations in materials physics, Teaching Asssistant, (Supervised 2 students projects) (~40 h)
- Apr.-Jul. 2023, Theoretical materials physics, Teaching Asssistant, (~30 h)

Teaching Assistance, Friedrich-Alexander-University of Erlangen-Nürnberg (16.04.2018 – 15.04.2022)

- Pre-course MatLab/Octave and Linux
- Introduction to atomistic simulation methods
- Computational Nanoscience
- Thermodynamics and mechanics of materials
- Numerical Methodes in Materials Science and Engineering
- Student exams handling and supervision

PEER-REVIEWED PUBLICATIONS

Published and submitted:

1. Pressure-driven Homogenization of Lithium Disilicate Glasses. Y. Bakhouch, S. Buchner, R. A. Silveira, L. Resende, A. S. Pereira, A. Hasnaoui, **A. Atila,** *Journal of American Ceramic Society*, (2024), DOI: 10.1111/jace.19778

2. Sheared ice surfaces liquefy without much heating. **A. Atila**, S. Sukhomlinov, M. Müser (Submitted)

3. Icosahedral Connectivity and Medium-Range Structure in a Monoatomic Metallic Glass. A. Houba, M. El Ayoubi, A. Samiri, **A. Atila**, A. Hasnaoui (Submitted)

4. On the relationship between adsorption energy and surface chemistry in soda-lime silicate glasses, **A. Atila** (Submitted as invited paper)

5. The origins of phase separation in binary aluminosilicate glasses. H. Kharouji, A. Hasnaoui, **A. Atila** (Submitted)

6. Periodic linear complexions: Co-segregation of solutes at a low-angle grain boundary in a magnesium alloy. R. Pei, Z. Xie, **A. Atila**, S. Anoldi, L. Xiao, X. Liu, H. Wang, S. Korte-Kerzel, J. Guénolé, T. Al-Samman, DOI: arXiv:2310.11084 (To be submitted)

7. On the structure and icosahedral interconnectivity in Tantalum monoatomic glass produced under pressure. M. Kbirou, **A. Atila** , A. Hasnaoui (Submitted)

8. Atomistic origins of deformation-induced structural anisotropy in

metaphosphate glasses and its influence on mechanical properties. **A. Atila**, E. Bitzek, *Journal of Non-Crystalline Solids*, 627, 122822 (2024), DOI: 10.1016/j.jnoncrysol.2024.122822

9. Exploring Solute Behavior and Texture Selection in Magnesium Alloys at the Atomistic Level. F. Mouhib, Z. Xie, **A. Atila**, J. Guénolé, S. Korte-Kerzel, T. Al-Samman, *Acta Materialia*, 119677 (2024), DOI: 10.1016/j.actamat.2024.119677

10. Topology of Anisotropic Glasses from Persistent Homology Analysis. Z. Pan, **A. Atila**, E. Bitzek, L. Wondraczek, *Journal of Non-Crystalline Solids*, 627, 122801 (2024), DOI: 10.1016/j.jnoncrysol.2023.122801

11. Structural Origin of the Boson Peak in Silicate Glasses: Insight from Molecular Dynamics. A. El Hamdaoui, E.M. Ghardi, **A. Atila**, H. Jabraoui, M. Badawi, A. Hasnaoui, S. Ouaskit, *Physical Chemistry Chemical Physics*, 25 (2023), pp. 31270-31280, DOI: 10.1039/D3CP02912C

12. The Origin of Deformation-Induced Topological Anisotropy in Silica Glass. S. Ganisetti, **A. Atila**, J. Guénolé, A. Prakash, J. Horbach, L. Wondraczek, E. Bitzek, *Acta Materialia*, 257, 119108 (2023), DOI: 10.1016/j.actamat.2023.119108

13. Thermally activated nature of synchro-Shockley dislocations in Laves phases. Z. Xie, D. Chauraud, **A. Atila**, E. Bitzek, S. Korte-Kerzel, J. Guénolé, Scripta Materialia, 235, 115588 (2023), DOI: 10.1016/j.scriptamat.2023.115588

14. Unveiling the mechanisms of motion of synchro-Shockley dislocations. Z. Xie, D. Chauraud, **A. Atila**, E. Bitzek, S. Korte-Kerzel, J. Guénolé, *Physical. Review. Materials*, 7, 053605 (2023), DOI: 10.1103/PhysRevMaterials.7.053605

15. Density-diffusion relationship in soda-lime phosphosilicate. Y. Ouldhnini, **A. Atila**, S. Ouaskit, A. Hasnaoui, *Journal of Non-Crystalline Solids*, 590, 121665 (2022) DOI: 10.1016/j.jnoncrysol.2022.121665

16. Atomistic origins of the mixed-alkali effect in phosphosilicate glasses. **A. Atila**, Y. Ouldhnini, S. Ouaskit, A. Hasnaoui, *Physical. Review. B*, 105, 134101 (2022), DOI: 10.1103/PhysRevB.105.134101

17. Atomistic insights into the structure and elasticity of densified 45S5 bioactive glass. Y. Ouldhnini[*], **A. Atila**[*], S. Ouaskit, A. Hasnaoui,

[*] Joint first author

Physical Chemistry Chemical Physics, 23 (28) (2021), pp. 15292-15301, DOI: 10.1039/D1CP02192C

18. On the Presence of Nanoscale Heterogeneity in $Ni_{15}Co_{15}Al_{70}$ Metallic Glass Under Pressure. **A. Atila***, M. Kbirou*, S. Ouaskit, A. Hasnaoui, *Journal of Non-Crystalline Solids*, 550, 120381 (2020), DOI: 10.1016/j.jnoncrysol.2020.120381

19. Atomic structure and modifiers clustering in silicate glasses: Effect of modifier cations. **A. Atila**, DOI : arXiv:2007.09247

20. Ionic self-diffusion and the glass transition anomaly in aluminosilicates. **A. Atila**, S. Ouaskit, A. Hasnaoui, Physical. Chemistry. Chemical. Physics. 22 (30) (2020), pp. 17205-17212, DOI: 10.1039/D0CP02910F

21. Atomistic insights into the impact of charge balancing cations on the structure and properties of aluminosilicate glasses. **A. Atila**, M. Ghardi, A. Hasnaoui, S. Ouaskit, *Physical. Review. B*, 100, 144109 (2019), DOI: 10.1103/PhysRevB.100.144109

22. Alumina effect on the structure and properties of calcium aluminosilicate in the percalcic region: A molecular dynamics investigation. **A. Atila**, M.Ghardi, A. Hasnaoui, S. Ouaskit, *Journal of Non-Crystalline Solids*, 525, 119470 (2019), DOI: 10.1016/j.jnoncrysol.2019.119470

23. Computational Insights into the Structure of Barium Titanosilicate Glasses. E.M. Ghardi, **A. Atila**, M. Badawi, A. Hasnaoui, S. Ouaskit, *Journal of American Ceramic Society*, 102, 6626 (2019), DOI: 10.1111/jace.16536

INVITED TALKS

"Atomistic simulations of oxide glasses". FPDK, Khouribga, Morocco

PRESENTATIONS, POSTERS, AND WORKSHOPS

Talk, " Plasticity in fragile and strong bulk metallic glasses during nanoindentation."**A. Atila**, Sergey Sukhomlinov, and Martin Müser. USTV-DGG joint meeting, Orléans, France, 22-24.05.2023.

Talk, "The Origin of Deformation-Induced Topological Anisotropy in Silica Glass." S. Ganisetti, **A. Atila**, J. Guénolé, A. Prakash, J. Horbach, L. Wondraczek, and E. Bitzek. International Congress on Glass ICG2022, Berlin, Germany, 03-8.07.2022.

Under line: Corresponding author

Talk, "Topology-Controlled Deformation Behavior of Oxide Glasses." **A. Atila** and E. Bitzek. DPG spring meeting, Regensburg, Germany, 06-11.03.2022 (Postponed due to COVID-19).

IBM: ML0101EN, Machine Learning with Python: A Practical Introduction. 08.2020.

Talk, "Atomistic Study of Mechanical and Structural Anisotropy in Metaphosphate Glasses." **A. Atila** and E. Bitzek. USTV-DGG joint meeting, Orléans, France, 15-19.06.2020 (Cancelled due to COVID-19).

Poster, "Atomistic mechanisms of Crack Nucleation in Silicate Glasses." **A. Atila** and E. Bitzek. USTV-DGG joint meeting, Orléans, France, 15-19.06.2020 (Cancelled due to COVID-19).

Poster, "Atomic-Scale Study of Deformation-Induced Topological Anisotropy in Silica and Metaphosphate Glasses." **A. Atila**, S. Ganisetti, J. Guénolé, A. Prakash, J. Horbach, L. Wondraczek, and E. Bitzek. 4th Int. Workshop on Glass & Entropy, Jena, Germany, 9-12.09.2019.

Talk, "Atomistic Study of Mechanical and Structural Anisotropy of Metaphosphate Glasses." **A. Atila** and E. Bitzek. ISAM^4 Symposium, Erlangen, Germany, 5-8.08.2019.

Poster, "Mixed alkaline-earth effect in metaphosphate glasses". **A. Atila** and E. Bitzek. DGG conference, Nürenberg, Germany, 13-15.05.2019.

Poster, "Structural and mechanical properties of sodium, magnesium and calcium metaphosphate glasses: insights from molecular dynamics simulations." **A. Atila** and E. Bitzek. DPG spring meeting, Regensburg, Germany, 1-5.04. 2019.

Poster, "Atomistic simulations of silica and metaphosphate glasses: mechanical properties and mechanically-induced structural anisotropy." **A. Atila**, S. Ganisetti, and E. Bitzek. SPP1594 Spring school "Glass under load" Dusseldorf, Germany, 19-22.02. 2019.

Poster, “The role of disorder in the BaO-TiO_2-SiO_2 glass plasticity: a molecular dynamics study”. EM. Ghardi, **A. Atila**, A. Hasnaoui and S. Ouaskit. 9ème Rencontre nationale des jeunes chercheurs en physique in Casablanca, Morocco 27-29.12.2018.

Paris International School on Advanced Computational Material Science – PISACMS2018, Paris, France, 26.08-2.09.2018.

Talk, "Alumina content effect on thermodynamic mechanical and structural properties of calcium silicate glass: a molecular dynamics simulation." **A. Atila**, A. Hasnaoui and S. Ouaskit. 6th International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-21.03.2018.

Poster, "Charge balancing cations effect on elastic moduli of aluminosilicate glasses revealed by molecular dynamics simulations." **A. Atila**, EM. Ghardi, A. Hasnaoui and S. Ouaskit. 6th International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-21.03.2018.

Poster, "Structural investigation of TiO_2 role in barium titanosilicate glasses: A molecular dynamics simulation". EM. Ghardi, **A. Atila**, A. Hasnaoui and S. Ouaskit. 6th International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-22.03.2018.

Poster, "Molecular dynamic study of the thermodynamic and structural properties of Calcium Aluminosilicate glass." **A. Atila**, A. Hasnaoui and S. Ouaskit. 2sd International conference of functional materials and their technological applications (CIMFAT). Casablanca, Morocco, on 13.10.2017.

PROFESSIONAL SERVICE

Member of the organization committee.
6th International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-21.03.2018.

Member of the organization committee.
1st International Conference on Theoretical and High Energy Physics (ICTHP), Casablanca, Morocco, 22-24.09.2016.

REFEREE SERVICE

Acta Materialia,
Scientific Reports,
Journal of Non-Crystalline Solids,
Journal of Non-Crystalline Solids: X,
Journal of Molecular Liquids,
Journal of Physics and Chemistry of Solids,
Modelling and Simulation in Materials Science and Engineering,
Journal of Applied Physics,
Applied Physics Letters,
Journal of Physical Chemistry,
Journal of Materials Science,
Physica Scripta,
Vacuum,
Journal of Inorganic and Organometallic Polymers and Materials

LANGUAGES	**English, French, Arabic:** Full professional proficiency **German:** Beginner (A1 level)
COMPUTER SKILLS	• **Simulations**: Classical & Reactive MD (LAMMPS), DFT (Quantum Espresso). • **Programming**: Python, FORTRAN, C/C++ • **Scientific publishing**: LaTeX • **Software**: MS Office • **OS**: Windows, Linux (system administration) • **Plotting**: GNUPLOT, Matplotlib, Origin.