

## ACHRAF ATILA

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

### EDUCATION

**PhD Friedrich-Alexander-University of Erlangen-Nürnberg, (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

**Research Associate, Universität des Saarlandes (01.07.2022 – )**

### EXPERIENCE

**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: 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 Mcoreh

### TEACHING

### EXPERIENCE

**Teaching Assistance, Universität des Saarlandes (01.07.2022 – )**

**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

- Teaching assistant in the lectures “Computational Nanoscience”, “Thermodynamics and mechanics of materials” and “Numerische Methoden in den Werkstoffwissenschaften”
- Student exams handling and supervision

## PEER-REVIEWED PUBLICATIONS

### ***Published:***

1. Thermally activated nature of synchro-Shockley dislocations in Laves phases. Z. Xie, D. Chauraud, **A. Atila**, E. Bitzek, S. Korte-Kerzel, J. Guénolé, *Submitted*, DOI: [10.48550/arXiv.2303.03044](https://doi.org/10.48550/arXiv.2303.03044) (Submitted to Scripta Materialia)
2. 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 (Submitted)
3. The Origin of Deformation-Induced Topological Anisotropy in Silica Glass. S. Ganisetti, **A. Atila**, J. Guénolé, A. Prakash, J. Horbach, L. Wondraczek, E. Bitzek, *Submitted*, DOI: [10.48550/arXiv.2206.03039](https://doi.org/10.48550/arXiv.2206.03039)
4. 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](https://doi.org/10.1103/PhysRevMaterials.7.053605)
5. 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](https://doi.org/10.1016/j.jnoncrysol.2022.121665)
6. 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](https://doi.org/10.1103/PhysRevB.105.134101)
7. Atomistic insights into the structure and elasticity of densified 45S5 bioactive glass. Y. Ouldhnini\*, A. Atila\*, S. Ouaskit, A. Hasnaoui, *Physical. Chemistry. Chemical. Physics*. 23 (28) (2021), pp. 15292-15301, DOI: [10.1039/D1CP02192C](https://doi.org/10.1039/D1CP02192C)
8. On the Presence of Nanoscale Heterogeneity in Ni<sub>15</sub>Co<sub>15</sub>Al<sub>70</sub> 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](https://doi.org/10.1016/j.jnoncrysol.2020.120381)

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\* Joint first author

Under line: Corresponding author

9. 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](https://doi.org/10.1039/D0CP02910F)
10. 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](https://doi.org/10.1103/PhysRevB.100.144109)
11. 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](https://doi.org/10.1016/j.jnoncrysol.2019.119470)
12. 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](https://doi.org/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.

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. 4<sup>th</sup> 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<sup>4</sup> Symposium, Erlangen, Germany, 5-8.08.2019.

Poster, "Mixed alkaline-earth effect in metaphosphate glasses". A. Atila and E. Bitzek. DGG conference, Nürnberg, 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<sub>2</sub>-SiO<sub>2</sub> glass plasticity: a molecular dynamics study". EM. Ghardi, A. Atila, A. Hasnaoui and S. Ouaskit. 9<sup>ème</sup> 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. 6<sup>th</sup> International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6<sup>th</sup>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. 6<sup>th</sup> International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-21.03.2018.

Poster, "Structural investigation of TiO<sub>2</sub> role in barium titanosilicate glasses: A molecular dynamics simulation". EM. Ghardi, **A. Atila**, A. Hasnaoui and S. Ouaskit. 6<sup>th</sup> 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. 2<sup>sd</sup> International conference of functional materials and their technological applications (CIMFAT). Casablanca, Morocco, on 13.10.2017.

**PROFESSIONAL  
SERVICE**

**Member of the organization committee.**

6<sup>th</sup> International Conference Franco-Maghrebine on Nanomaterials for Energy and Environment (6'CFMNEE), Casablanca, Morocco, 19-21.03.2018.

**Member of the organization committee.**

1<sup>st</sup> 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**

- **Programming:** Python, FORTRAN, C/C++
- **Scientific publishing:** LaTeX
- **Software:** MS Office
- **OS:** Windows, Linux (system administration)

- **Plotting:** GNUPLOT, Origin.
- **Simulations:** Classical & Reactive MD (LAMMPS), DFT (Quantum Espresso).