

# Prof. Dr. Nina Merkert (née Gunkelmann)

## Publications

1. S. Chakrabarty, D. A. De Abreu, I. A. Alhafez, O. Fabrichnaya, N. Merkert, A. Schnickmann, T. Schirmer, U. E. A. Fittschen, M. Fischlschweiger, Kinetics of  $\gamma$ -LiAlO<sub>2</sub> Formation out of Li<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub> Melt—A Molecular Dynamics-Informed Non-Equilibrium Thermodynamic Study *Solids* 5:561, DOI: 10.3390/solids5040038, 2024.
2. M. Shaban, N. Merkert, A. C. T. van Duin, D. van Duin, A. P. Weber. Advancing DBD Plasma Chemistry: Insights into reactive nitrogen species (RNS) such as NO<sub>2</sub>, N<sub>2</sub>O<sub>5</sub>, and N<sub>2</sub>O Optimization and Species Reactivity through Experiments and Molecular Dynamics Simulations. *Environ. Sci. Technol.* 58(36):16087, DOI: 10.1021/acs.est.4c04894, 2024.
3. S. Hampel, I. A. Alhafez, A. Schnickmann, S. Wunderlich, H. Li, M. Fischlschweiger, T. Schirmer, N. Merkert, U. E. A. Fittschen. Experimental and Simulation Studies on the Mn Oxidation State Evolution of a Li<sub>2</sub>O-MnO<sub>x</sub>-CaO-SiO<sub>2</sub> Slag Analogue. *Minerals* 14(9):868, 2024.
4. D. Thürmer, O. R. Deluigi, H. M. Urbassek, E. M. Bringa, N. Merkert. Atomistic Simulations of the Shock and Spall Behavior of the Refractory High-Entropy Alloy HfNbTaTiZr. *High Entropy Alloys & Materials*, DOI: 10.1007/s44210-024-00042-2, 2024.
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6. U. E. A. Fittschen, S. Hampel, T. Schirmer, N. Merkert. Multimodal spectroscopy and molecular dynamic simulations to understand redox-chemistry and compound formation in pyrometallurgical slags: example of manganese oxidation state with respect to lithium recycling. *Appl. Spectrosc. Rev.*, DOI: 10.1080/05704928.2024.2350988, 2024.
7. I. A. Alhafez, O. R. Deluigi, D. Tramontina, N. Merkert, H. M. Urbassek, E. M. Bringa. Nanoindentation into a bcc high-entropy HfNbTaTiZr alloy – an atomistic study of the effect of short-range order. *Sci. Rep.* 14:9112, 2024.
8. D. Thürmer, H.-T. Luu, N. Merkert. Molecular dynamics simulation of shock waves in Fe and Fe–C: Influence of system characteristics. *J. Appl. Phys.* 135:155901, 2024.
9. L. Hahn, S. A. Blaue, P. Höhn, N. Merkert, P. Klein. Open Educational Resources für den Hochschulbereich. In *PhyDid B, Didaktik der Physik, Beiträge zur virtuellen DPG-Frühjahrstagung*. Ed: H. Grötzebauch, S. Heinicke, 2023.
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11. G.S. Dutta, D. Meiners, N. Merkert. A Study of Free-Form Shape Rationalization Using Biomimicry as Inspiration. *Polymers* 15:2466, 2023.

12. S. Raumel, K. Barianti, H.-T. Luu, N. Merkert, F. Dencker, F. Nürnberger, H.J. Maier, M. C. Wurz. Characterization of the tribologically relevant cover layers formed on copper in oxygen and oxygen-free conditions. *Friction*, DOI: 10.1007/s40544-022-0695-5, 2023.
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15. D. Thürmer, N. Gunkelmann. Shock-induced spallation in a nanocrystalline high-entropy alloy: An atomistic study. *J. Appl. Phys.* 131:065902, 2022.
16. D. Thürmer, S. Zhao, O. R. Deluigi, C. Stan, I. A. Alhafez, H. M. Urbassek, M. A. Meyers, E. M. Bringa, N. Gunkelmann. Exceptionally high spallation strength for a high-entropy alloy demonstrated by experiments and simulations. *J. Alloys Compd.* 895:162567, 2022.
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26. H.-T. Luu, R. G. A. Veiga, N. Gunkelmann. Atomistic Study of the Role of Defects on  $\alpha \rightarrow \epsilon$  Phase Transformations in Iron under Hydrostatic Compression. *Metals* 9(10):1040, 2019, **Journal issue cover image, Volume 9, Issue 10.**
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