# Prof. Dr. Nina Merkert (née Gunkelmann)

# Publications

1. I. A. Alhafez, O. R. Deluigi, D. Tramontina, F. Valencia, N. Merkert, D. Farkas, A. Caro, H. M. Urbassek, E. M. Bringa. Nanoindentation into a dual-phase bicontinuous lamellar high-entropy alloy. *J. Mater. Res. Technol. 37:1406*, DOI: 10.1016/j.jmrt.2025.05.257, 2025.

2. H.-T. Luu, N. Merkert. Investigation of solid-state diffusion bonding of Al–Cu interfaces of metal joints using molecular dynamics simulations. *Results Surf. Interfaces 20:100574*, DOI: 10.1016/j.rsurfi.2025.100574, 2025.

3. 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 $\gamma$-$LiAlO_2$ Formation out of $Li_2O$-$Al_2O_3$ Melt—A Molecular Dynamics-Informed Non-Equilibrium Thermodynamic Study *Solids 5:561*, DOI: 10.3390/solids5040038, 2024.

4. 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 $NO_2$, $N_2O_5$, and $N_2O$ Optimization and Species Reactivity through Experiments and Molecular Dynamics Simulations. *Environ. Sci. Technol. 58(36):16087*, DOI: 10.1021/acs.est.4c04894, 2024.

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8. 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.

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10. 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.

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