

Jun. Prof. Dr. Nina Merkert (née Gunkelmann)

Publications

1. 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.*, DOI: 10.1021/acs.est.4c04894, 2024.
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3. 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.
4. S. Hampel, I. A. Alhafez, T. Schirmer, N. Merkert, S. Wunderlich, A. Schnickmann, H. Li, M. Fischlschweiger, U. E. A. Fittschen. Engineering Compounds for the Recovery of Critical Elements from Slags: Melt Characteristics of Li_5AlO_4 , LiAlO_2 , and LiAl_5O_8 . *ACS Omega*, DOI: 10.1021/acsomega.4c00723, 2024.
5. 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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7. 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.
8. 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.
9. A. Demirci, D. Steinberger, M. Stricker, N. Merkert, D. Weygand, S. Sandfeld. Statistical analysis of discrete dislocation dynamics simulations: initial structures, cross-slip and microstructure evolutions. *MSMSE* 31:075003, 2023.
10. G.S. Dutta, D. Meiners, N. Merkert. A Study of Free-Form Shape Rationalization Using Biomimicry as Inspiration. *Polymers* 15:2466, 2023.
11. 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.

12. S. Homann, H.-T. Luu, N. Merkert. Molecular dynamics simulations of the machining of oxidized and deoxidized titanium work pieces. *Results Surf. Interfaces* 9:100085, 2022.
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14. D. Thürmer, N. Gunkelmann. Shock-induced spallation in a nanocrystalline high-entropy alloy: An atomistic study. *J. Appl. Phys.* 131:065902, 2022.
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25. 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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