Liste der Veröffentlichungen zum Verwendungsnachweis
3xa-Projekt

Vorhabensbezeichnung:	3xa Exascale-Simulationssoftware für Systeme mit Dreikörperwechelwirkungen
Laufzeit des Vorhabens:	01.11.2022 bis 31.12.2025

HLRS

Söhner, M., Niethammer, C. "MPPI - Type safe C++ Datatypes for MPI". *Proceedings of the SC '25 Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis. SC Workshops '25*, 439–448, 2025. https://doi.org/10.1145/3731599.3767390

HSU/HPC

Pinzon Escobar, J.A., Hocks, A., Neumann, P. "Node-Level Performance of Adaptive Resolution in ls1 Mardyn". In: Paszynski, M., et al. (Hrsg.) *Computational Science – ICCS 2025 Workshops*. ICCS 2025. Lecture Notes in Computer Science, Bd. 15911. Springer, Cham. https://doi.org/10.1007/978-3-031-97570-7_4

Pinzon Escobar, J.A., Mühlhäußer, M., Bungartz, H.J., Neumann, P. "Linked cell traversal algorithms for three-Body interactions in molecular dynamics". *Computer Physics Communications*, Bd. 321 (2026), S. 110028. https://doi.org/10.1016/j.cpc.2026.110028

Pinzon Escobar, J.A., Neumann, P. "Adaptive Resolution Scheme for Non-additive Molecular Three-Body Potentials". *Akzeptierte Einreichung: ICCS 2026 (Full Paper).*

HSU/LTD

Marienhagen, P., Meier, K. "Calculation of thermodynamic properties using path integral Monte Carlo simulations in the canonical ensemble". *J. Chem. Phys.* 163, 074116 (2025). https://doi.org/10.1063/5.0282863 (Editor's pick, 2025 JCP Emerging Investigators Special Collection).

Marienhagen, P., Meier, K. "Calculation of thermodynamic properties of neon using path integral Monte Carlo simulations and *ab initio potentials*". *In Vorbereitung, geplante Einreichung: J. Chem. Phys. 2026 (Full Paper).*

Sui, M., Marienhagen, P., Duffek, J., Neumann, P., Meier, K. "Efficient implementation of nonadditive three-body *ab initio* potentials for Monte Carlo simulations". *In Vorbereitung, geplante Einreichung: J. Chem. Theory Comput. 2026 (Full Paper).*

TUB

Nitzke, I., Guevara-Carrion, G., Saric, D., Homes, S., Stephan, S., Fingerhut, R., Bernreuther, M., Hasse, H., and Vrabec, J. "ms2: A molecular simulation tool for thermodynamic properties, release 5.0". *Comput. Phys. Commun.*, 109541, 2025.

Mace, E., Vrabec, J. "Thermodynamic properties of ammonia-water mixtures in the vapor-liquid, critical, and Widom regions". *J. Chem. Phys.*, 163(18):184305, 2025.

Nitzke, I., Vrabec, J. “Numerical Discrimination of Thermodynamic Monte Carlo Simulations in All Eight Statistical Ensembles”. *J. Chem. Theory Comput.*, 19(12):3460–3468, 2023.

TUM

Pinzon Escobar, J.A., Mühlhäußer, M., Bungartz, H.J., Neumann, P. “Linked cell traversal algorithms for three-Body interactions in molecular dynamics”. *Computer Physics Communications*, Bd. 321 (2026), S. 110028. https://doi.org/10.1016/j.cpc.2026.110028

Mühlhäußer, M., Newcome, S., Mishra, M., Schuhmacher, J., Bungartz, H.J. “Tuning Three-Body Performance in AutoPas - Evaluating Shared-Memory Algorithms for Three-Body Interactions in Molecular Dynamics”. *In Vorbereitung, geplante Einreichung: Computer Physics Communications 2026 (Full Paper)*.