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MACE Force Field Models for the Periodic Table

I will report on our latest efforts to create universally applicable machine learning force fields using the MACE architecture. Large publicly available databases (such as OMAT and OMOL) and large scale GPU compute allow the construction of force field models that cover most of the periodic table and are suitable out of the box for exploration tasks, and in some cases (e.g. organic molecules) for accurate production level simulations. Fine tuning material models with very little effort yields near-DFT accuracy. The latest models, such as MACE-POLAR-1 include electrostatic interactions with some notion of self-consistency.



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www.iwr.uni-heidelberg.de/en/events/colloquium-gabor-csanyi-2026