The most important publications

1. Erlebach, A., Nachtigall, P., **Grajciar, L**., (2022): Accurate large-scale simulations of siliceous zeolites by neural network potentials. In: *npj Computational Materials*, 8, 174. IF = 12.256

   We developed a **linear scaling reactive machine learning potential (MLP) for general potential surface modelling of silica** covering a broad range of silica densities from siliceous zeolites with large pores through denser zeolitic frameworks and silica glass towards very dense silica polymorphs. It covered broad range of configurational space including not only structures close to equilibria both also non-equilibrium structures necessary for description of bond-breaking events. The resulting **MLP retains the accuracy of DFT** calculations across the complex zeolitic classes considered, **outperforming specialized analytical force fields for silica by order(s) of magnitude in accuracy**, while **speeding up the calculations in comparison to DFT by at least three orders of magnitude**. We applied this MLP for high-throughput reoptimization of the existing zeolite databases and **revealed more than twenty thousand additional hypothetical zeolites within the synthetic feasibility range** providing essential input for the future screening studies on structure-property correlations in zeolites. This work represented a proof-of-principle study, which we are now following by development of MLPs for more complex and truly realistic systems such as aluminosilicate zeolites in reactive interaction with the water solution (*10.26434/chemrxiv-2022-d1sj9*) and which inch us closer towards the ultimate goal of computer-aided design and discovery of zeolites. *I conceived, planned, and coordinated the study, co-drafted the manuscript and acted as a senior corresponding author.*

2. Heard, C.J., **Grajciar, L**., Rice, C.M., Pugh, S.M., Nachtigall, P., Ashbrook, S., Morris, R.E., (2019): Fast Room Temperature Lability of Aluminosilicate Zeolites. In: *Nature Communications*, 10 (1), 1-7. IF = 17.7

   In this work, we showed, combining biased ab initio molecular dynamics with advanced solid state NMR (carried out by our experimental colleagues), that **even at room temperature zeolites show significant, fast lability of their bonds when in contact with liquid water**. This challenges the **conventional view of zeolites as static entities under mild condition** and will be of great importance to our understanding of low temperature interactions with water in evolving fields such as bio-refinery catalysis or in synthetic manipulations enabling access to new zeolitic materials (such the ADOR process 10.1038/NCHEM.1662 on which I also collaborated). *I identified new mechanistic routes for zeolite lability in water using open-ended searches with biased ab initio molecular dynamics (initially for germanosilicate zeolites - work on which was published later with my as a corresponding author - 10.1021/acs.jpcc.1c06873), motivated the experimental investigation and co-drafted the manuscript.*

3. Grajciar, L. (2015): Low-memory iterative density fitting. In: *Journal of Computational Chemistry*, 36, 1521-1535. *The article featured on the cover of the Issue 20*. IF = 3.672

   An implementation of a preconditioned conjugate gradient solver for a specific linear system of equation encountered in density functional theory calculations – the density fitting equations. Optimized implementation in the industry-leading TURBOMOLE quantum chemistry program package led to **order-of-magnitude savings in memory consumption** and enabled treatment of **large molecules (few thousand atoms) on a single multicore** processor workstation with no accuracy loss and only negligible additional costs.