

Publication list and the list of other scientific results

1. International publications with peer review process

1. Šípka, M., Erlebach, A., **Grajciar, L.**, (2023): Constructing collective variables using invariant learned representations. In: *Journal of Chemical Theory and Computation*, 10.1021/acs.jctc.2c00729. IF= 6.006
2. 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
3. Jin, M., Liu, M., Nachtigall, P., **Grajciar, L.**, Heard, C.J., (2021): Mechanism of Zeolite Hydrolysis under Basic Conditions. In: *Chemistry of Materials*, 33, 9202-9212. IF = 10.508
4. Jin, M., Veselý, O., Heard, C.J., Kubů, M., Nachtigall, P., Čejka, J., **Grajciar, L.**, (2021): The Role of Water Loading and Germanium Content in Germanosilicate Hydrolysis. In: *Journal of Physical Chemistry C*, 125, 23744-23757. IF = 4.177
5. Li, S., He, J., **Grajciar, L.**, Nachtigall, (2021): Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling. In: *Journal of Materials Chemistry C*, 9, 11132-11141. IF = 8.067
6. Li, S., He, J., Nachtigall, P., **Grajciar, L.**, Brivio, F., (2021): Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS₄) nanowires with carriers induces half-metallicity. In: *Journal of Materials Chemistry C*, 9, 3122-3128. IF = 8.067
7. Hou, D., **Grajciar, L.**, Nachtigall, P., Heard, C.J., (2020): Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum. In: *ACS Catalysis*, 10 (19), 11057-11068. IF = 13.7
8. Heard, C.J., **Grajciar, L.**, Uhlik, F., Shamzy, M., Opanasenko, M., Čejka, J., Nachtigall, P., (2020): Zeolite (In)Stability under Aqueous or Steaming Conditions In: *Advanced Materials*, 2003264. IF = 32.086 (**Review article**)
9. Liu, M., Veselý, O., Eliášová, P., Shamzhy, M., Lyu, P., **Grajciar L.**, (2020): Identification of the Most Active Sites for Tetrahydropyranlation in Zeolites: MFI as a test case. In: *Catalysis Today*, 345, 156-174. IF = 6.562
10. 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
11. Li, S., He, J., Nachtigall, P., **Grajciar, L.**, Brivio, F., (2019): Control of Spintronic and Electronic Properties of Bimetallic and Vacancy-ordered Vanadium Carbide MXenes via Surface Functionalization. In: *Physical Chemistry Chemical Physics*, 21 (46), 25802-25808. IF = 3.945
12. Lyu, P., Ertl, M., Heard, C.J., **Grajciar, L.**, Radha, A.V., Martin, T., Breu, J., Nachtigall, P., (2019): Structure Determination of the Oxygen Evolution Catalyst Mossbaurite. In: *Journal of Physical Chemistry C*, 123 (41), 25157-25165. IF = 4.177
13. Heard, C. J., **Grajciar, L.**, Nachtigall, P., (2019): The Effect of Water on the Validity of Loewenstein's Rule. In: *Chemical Science*, 10 (22), 5705-5711. IF = 9.969
14. Thang, H.V., Vaculík, J., Přeč, J., Kubů, M., Čejka, J., Nachtigall P., Bulánek, R., **Grajciar, L.**, (2019): The Brønsted acidity of three- and two-dimensional zeolites. In: *Microporous and Mesoporous Materials*, 282, 121-132. IF = 5.876
15. **Grajciar, L.**, Heard, C. J., Bondarenko, A. A., Polynski, M. V., Meeprasert, J., Pidko E. A., Nachtigall, P., (2018): Towards operando computational modelling in heterogeneous catalysis. In: *Chemical Society Reviews*, 47, 8307-8348. IF = 60.615 (**Review article**)
16. Thang, H.V., Nachtigall P., **Grajciar, L.**, (2018): The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology. In: *Catalysis Today*, 304, 12-21. IF = 6.562
17. **Grajciar, L.** (2016): PbS clusters embedded in the sodalite zeolite cavity of different composition: unraveling the structural evolution and optical properties using ab initio calculations. In: *Journal of Physical Chemistry C*, 120, 27050-27065. IF = 4.177
18. Lazarski, R., Burow, A. M., **Grajciar, L.**, Sierka, M., (2016): Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Analytical gradients. In: *Journal of Computational Chemistry*, 37, 2518-2526. IF = 3.672
19. **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

20. **Grajciar, L.**, Nachtigall, P., Bludsky, O., Rubes, M. (2015): Accurate ab initio description of adsorption on coordinatively unsaturated Cu²⁺ and Fe³⁺ sites in MOFs. In: *Journal of Chemical Theory and Computation*, 11, 230-238. IF = 6.006
21. Thang, H. V., **Grajciar, L.**, Nachtigall, P., Bludsky, O., Arean, C. O., Frydova, E., Bulanek, R. (2014): Adsorption of CO₂ in FAU zeolites: Effect of zeolite composition. In: *Catalysis Today*, 227, 50-56. IF = 6.562
22. Roth, W. J., Nachtigall, P., Morris, R. E., Wheatley, P. S., Ashbrook, S. E., Seymour, V., Chlubna, P., **Grajciar, L.**, Polozij, M., Zukal, A., Shvets, O., Cejka, J. (2013): A family of complex zeolites with controlled pore size prepared through a 'top down' method. In: *Nature Chemistry*, 5, 628-633. IF = 24.274
23. Rubes, M., Wiersum, A. D., Llewellyn, P. L., **Grajciar, L.**, Bludsky, O., Nachtigall, P. (2013): Adsorption of propane and propylene on CuBTC MOF: Combined theoretical and experimental investigation. In: *Journal of Physical Chemistry C*, 117, 11159-11167. IF = 4.177
24. **Grajciar, L.**, Bludský, O., Roth, W. J., Nachtigall, P. (2013): Theoretical investigation of layered zeolite frameworks: Interaction between IPC-1P layers derived from zeolite UTL. In: *Catalysis Today*, 204, 15-21. IF = 6.562
25. Rubes, M., **Grajciar, L.**, Bludsky, O., Wiersum, A. D., Llewellyn, P. L., Nachtigall, P. (2012): Combined theoretical and experimental investigation of CO adsorption on coordinatively unsaturated sites in CuBTC MOF. In: *ChemPhysChem*, 13, 488-495. IF = 3.520
26. Nachtigall, P., **Grajciar, L.**, Perez-Pariente, J., Pinar, A. B., Zukal, A., Cejka, J. (2012): Control of CO₂ adsorption heats by the Al distribution in FER zeolites: Effect of synthesis conditions. In: *Physical Chemistry Chemical Physics*, 14, 1117-1120. IF = 3.945
27. **Grajciar, L.**, Cejka, J., Zukal, A., Arean, C. O., Palomino, G. T., Nachtigall, P. (2012): Controlling the adsorption enthalpy of CO₂ in zeolites by framework topology and composition. In: *ChemSusChem*, 5, 2011-2022. IF = 9.140
28. Chen, L., **Grajciar, L.**, Nachtigall, P., Duren, T. (2011): Accurate prediction of methane adsorption in a metal-organic framework with unsaturated metal sites by direct implementation of an ab initio derived potential energy surface in GCMC simulation. In: *Journal of Physical Chemistry C*, 115, 23074-23080. IF = 4.177
29. Kysilka, J., Rubes, M., **Grajciar, L.**, Nachtigall, P., Bludsky, O. (2011): Accurate description of argon and water adsorption on surfaces of graphene-based carbon allotropes. In: *Journal of Physical Chemistry A*, 115, 11387-11393. IF = 2.944
30. **Grajciar, L.**, Wiersum, A. D., Llewellyn, P. L., Chang, J-S., Nachtigall, P. (2011): Understanding CO₂ adsorption in CuBTC MOF: Comparing combined DFT-ab initio calculations with microcalorimetry experiments. In: *Journal of Physical Chemistry C*, 115, 17925-17933. IF = 4.177
31. **Grajciar, L.**, Bludsky, O., Nachtigall, P. (2010): Water adsorption on coordinatively unsaturated sites in CuBTC MOF. In: *Journal of Physical Chemistry Letters*, 1, 3354-3359. IF = 6.888
32. **Grajciar, L.**, Arean, C. O., Pulido, A., Nachtigall, P. (2010): Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER. In: *Physical Chemistry Chemical Physics*, 12, 1497-1506. IF = 3.945
33. Nachtigall, P., Bludsky, O., **Grajciar, L.**, Nachtigallova, D., Delgado, M. R., Arean, C. O. (2009): Computational and FTIR spectroscopic studies on carbon monoxide and dinitrogen adsorption on a high-silica H-FER zeolite. In: *Physical Chemistry Chemical Physics*, 11, 791-802. IF = 3.945

4. Book chapters

1. **Grajciar, L.**, Rubes, M., Bludsky, O., Nachtigall, P. (2015): Accurate ab initio description of adsorption on coordinatively unsaturated sites in MOFs In: *Metal-organic frameworks: materials modeling towards engineering applications*. CRC Press, Taylor & Francis Group Boca Raton, FL, USA, pp. 175-206.

7. Invited lectures

- 09/2021 Workshop on "Water in Zeolites". Liblice, Czechia. "Reactive Neural Network Potentials for Zeolites (and Water) with DFT Accuracy". (<https://water2020.katalyza.cz>)
- 06/2021 Institute for Institut für Chemie Quantenchemie der Festkörper/ Katalyse, Humboldt University, Berlin. "Reactive Neural Network Potentials for Zeolites with DFT Accuracy". (<https://www.chemie.hu-berlin.de/de/forschung/quantenchemie/seminars>)

10. Theses

- 2013 L. Grajciar. "Quantum-chemical study of adsorption in microporous materials". PhD thesis, Charles University.

11. Funding/grants

- 2020-2022 Junior group leader research project (two postdocs and one PhD student), Charles University ([Primus/20/SCI/004](#)): *Computational catalysis goes operando* (principal investigator, total € 250.000)
- 2017-2019 Co-investigator (supervision of two PhD students) with experimental collaborator (Jiří Čejka) as principal investigator, Czech Science Foundation ([17-01440S](#)): *Engineering of advanced catalysts from modular parts* (co-investigator, total for my part € 90.000)
- 2015-2016 Deutsche Forschungsgemeinschaft (DFG) Grant No. 269386423 (<http://gepris.dfg.de/gepris/projekt/269386423>): *Efficient global structure optimization in confined spaces: development and applications for design of advanced materials* (principal investigator, total € 120.000)
- 2014 TURBOMOLE GmbH internal project: *Low memory iterative density fitting* (principal investigator, total € 60.000)

11. Other publications (preprints)

1. Saha, I., Erlebach, A., Nachtigall, P., Heard, C.J., **Grajciar, L.**, (2022): Reactive Neural Network Potential for Aluminosilicate Zeolites and Water: Quantifying the effect of Si/Al ratio on proton solvation and water diffusion in H-FAU. In: *ChemRxiv*, 10.26434/chemrxiv-2022-d1sj9.