

Full list of publications

2017

D. Ji*, X. Xu*, L. Jiang*, **S. Amirjalayer***, L. Jiang, Y. Zhen, Y. Zou, Y. Yao, H. Dong, J. Yu, H. Fuchs, W. Hu, "Surface polarity and self-structured nanogrooves collaborative oriented molecular packing for high crystallinity towards efficient charge transport", *J. Am. Chem. Soc.*, **2017**, 139, 2734. (* **Co-first-authors**)

E. Maltseva, **S. Amirjalayer**, W. J. Buma, "Vibrationally-resolved spectroscopic studies of electronically excited states of 1,8-naphthalic anhydride and 1,8-naphthalimide: a delicate interplay between one $\pi\pi^*$ and two $n\pi^*$ states", *Phys. Chem. Chem. Phys.* **2017**, 19, 5861.

G. Wang, A. Rühling, **S. Amirjalayer**, M. Knor, J. B. Ernst, H.-J. Gao, H.-Y. Gao, C. Richter, N. L. Doltsinis, F. Glorius, H. Fuchs, "Ballbot-type motion of N-heterocyclic carbenes on gold surfaces", *Nature Chemistry*, **2017**, 9, 152.

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S. Amirjalayer*, A. Cnossen, W. R. Browne, B. L. Feringa, W. J. Buma*, S. Woutersen*, "Direct observation of a dark state in the photocycle of a light-driven molecular motor", *J. Phys. Chem A*, **2016**, 120, 8606. (***Corresponding author**)

S. Amirjalayer*, R. Schmid, "Influence of Pore Dimension on the Host–Guest Interaction in Metal–Organic Frameworks" ", *J. Phys. Chem C*, **2016**, 120, 27319. (***Corresponding author**)

T. Suhina, **S. Amirjalayer**, B. Mennucci, S. Woutersen, M. Hilbers, D. Bonn, A. M. Brouwer, "Excited-State Decay Pathways of Molecular Rotors: Twisted Intermediate or Conical Intersection?", *J. Phys. Chem. Lett.*, **2016**, 7, 4285.

O. Díaz Arado, M. Luft, H. Mönig*, P. A. Held, A. Studer, **S. Amirjalayer***, H. Fuchs, "Understanding molecular self-assembly of a diol compound by considering competitive interactions", *Phys. Chem. Chem. Phys.* **2016**, 18, 27390. (***Corresponding author**)

R. Becker, **S. Amirjalayer**, P. Li, S. Woutersen, J. N.H. Reek, "An iron-iron hydrogenase mimic with appended electron reservoir for efficient proton reduction in aqueous media", *Science Advances* **2016**, 2, e1501014.

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S. McMahon, **S. Amirjalayer**, Y. Halpin, W. J. Buma, S. Woutersen, C. Long, A. D. Rooney, M. T. Pryce, "Photochemistry and Electrochemistry of [(CO)₅MC(OMe)Me] (M = Cr or W) Explained Using Low-temperature Matrix Isolation, Picosecond Infrared Spectroscopy, Cyclic Voltammetry, and Time-dependent Density Functional Theory", *Dalton Trans.* **2015**, 44, 15424. (publication was selected for the **cover picture** Dalton Transactions Vol. 44 (35))

M. Knor, H.-Y. Gao, **S. Amirjalayer**, A. Studer, H. Fuchs, "Stereoselective formation of coordination polymers with 1,4-diaminonaphthalene on various Cu substrates", *Chem. Commun.* **2015**, 51, 10854.

A. Huerta-Viga, **S. Amirjalayer**, S. R. Domingos, H. Meuzelaar, A. Rupenyan, S. Woutersen, "Two-dimensional vibrational spectroscopy of Arg⁺...Glu⁻ salt bridges in peptides: Evidence for two distinct types of hydrogen-bond geometry", *J. Chem. Phys.* **2015**, 142, 212444.

E. M.M. Tan, **S. Amirjalayer**, S. Smolarek, A. Vdovin, F. Zerbetto, W. J. Buma, "Fast photodynamics of azobenzene probed by scanning excited state potential energy surfaces using slow spectroscopy", *Nature Commun.*, **2015**, 6:5860.

S. Bureekaew, V. Balwani, **S. Amirjalayer**, R. Schmid, "Isorecticular isomerism in 4,4-connected paddle-wheel metal-organic frameworks: structural prediction by the reverse topological approach", *CrystEngComm* **2015**, 17, 344.

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T. H. van der Loop, F. Ruesink, **S. Amirjalayer**, H. J. Sanders, W. Jan Buma, S. Woutersen, "Unraveling the Mechanism of a Reversible Photo-Activated Molecular Proton Crane", *J. Phys. Chem. B*, **2014**, 118, 12965.

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S. Amirjalayer, M. Tafipolsky, R. Schmid, "Surface Termination of the Metal-Organic Framework HKUST-1: A Theoretical Investigation", *J. Phys. Chem. Lett.*, **2014**, 5, 3206.

J. Conyard, I. A. Heisler, W. R. Browne, B. L. Feringa, **S. Amirjalayer***, W. J. Buma, S. Woutersen, S. R. Meech*, "Ultrafast Excited State Dynamics in 9,9'-Bifluorenylidene", *J. Phys. Chem. A*, **2014**, 118, 5961. (*corresponding author)

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A. Huerta-Viga, S. R. Domingos, **S. Amirjalayer**, S. Woutersen, "A salt-bridge structure in solution revealed by 2D-IR spectroscopy", *Phys. Chem. Chem. Phys.*, **2014**, 16, 15784.

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M. Wehring, P.C.M.M. Magusin, **S. Amirjalayer**, R. Schmid, F. Stallmach, "Ferrocene in the metal–organic framework MOF-5 studied by homo- and heteronuclear correlation NMR and MD simulation", *Micropor. Mesopor. Mater.*, **2014**, 186, 130.

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H. Noei, **S. Amirjalayer**, M. Müller, R. Schmid, M. Muhler, R. A. Fischer, Y. Wang, "Low-Temperature CO Oxidation over Cu-Based Metal–Organic Frameworks Monitored by FTIR Spectroscopy", *ChemCatChem*, **2012**, 4, 755. (Publication was selected for the **cover picture ChemCatChem** 6/2012)

S. Bureekaew, **S. Amirjalayer**, R. Schmid, "Orbital directing effects in copper and zinc based paddle-wheel metal organic frameworks: the origin of flexibility", *J. Mater. Chem.*, **2012**, 22, 10249.

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M. Tafipolsky, **S. Amirjalayer**, R. Schmid, "First-Principles-Derived Force Field for Copper Paddle-Wheel-Based Metal-Organic Frameworks", *J. Phys. Chem. C*, **2010**, 114, 14402.

M. Tafipolsky, **S. Amirjalayer**, R. Schmid, "Atomistic Theoretical Models for Nanoporous Hybrid Materials", *Micropor. Mesopor. Mater.*, **2010**, 129, 304. (**Invited review**).

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S. Amirjalayer, R. Schmid, "Conformational Isomerism in the Isoreticular Metal Organic Framework Family: A Force Field Investigation", *J. Phys. Chem. C*, **2008**, 112, 14980.

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