# AIMMS publication report for: 2021-04-12

### New papers: 2021-3/4

de Azevedo Santos, L., Ramalho, T. C., Hamlin, T. A., Bickelhaupt, F. M. **Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study** (Journal of Computational Chemistry, 15 Apr 2021)[https://doi.org/10.1002/jcc.26489]

Philippe, C., Bui, A. T., Batsongo-Boulingui, S., Pokladek, Z., Matczyszyn, K., Mongin, O., Lemiègre, L., Paul, F., Hamlin, T. A., Trolez, Y. **1,1,4,4-Tetracyanobutadiene-Functionalized Anthracenes: Regioselectivity of Cycloadditions in the Synthesis of Small Near-IR Dyes** (Organic letters, 19 Mar 2021)[https://doi.org/10.1021/acs.orglett.1c00136]

Rosato, M., Stringer, S., Gebuis, T., Paliukhovich, I., Li, K. W., Posthuma, D., Sullivan, P. F., Smit, A. B., van Kesteren, R. E. **Combined cellomics and proteomics analysis reveals shared neuronal morphology and molecular pathway phenotypes for multiple schizophrenia risk genes** (Molecular Psychiatry, Mar 2021)[https://doi.org/10.1038/s41380-019-0436-y]

Breedveld, G. D., Hansen, M. C., Hale, S. E., Allan, I. J., Hamers, T. **Effect of Extreme Weather Events on Contaminant Transport From Urban Run-Off to a Fjord System** (Frontiers in Environmental Science, Mar 2021)[https://doi.org/10.3389/fenvs.2021.601300]

Teusink, B., Kuipers, O. P., Moineau, S. **Symposium on Lactic Acid Bacteria-reading while waiting for a meeting** (FEMS Microbiology Reviews, Mar 2021)[https://doi.org/10.1093/femsre/fuaa049]

Hondius, D. C., Koopmans, F., Leistner, C., Pita-Illobre, D., Peferoen-Baert, R. M., Marbus, F., Paliukhovich, I., Li, K. W., Rozemuller, A. J., Hoozemans, J. J., Smit, A. B. **The proteome of granulovacuolar degeneration and neurofibrillary tangles in Alzheimer’s disease** (Acta Neuropathologica, Mar 2021)[https://doi.org/10.1007/s00401-020-02261-4]

Vermeeren, P., Zeist, W., Hamlin, T. A., Guerra, C. F., Bickelhaupt, F. M. **Not Carbon s–p Hybridization, but Coordination Number Determines C−H and C−C Bond Length** (Chemistry: A European Journal, 3 Mar 2021)[https://doi.org/10.1002/chem.202004653]

Svatunek, D., Hansen, T., Houk, K. N., Hamlin, T. A. **How the Lewis Base F– Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines** (The Journal of organic chemistry, 5 Mar 2021)[https://doi.org/10.1021/acs.joc.0c02963]

Wenzel, M., Dekker, M. P., Wang, B., Burggraaf, M. J., Bitter, W., van Weering, J. R., Hamoen, L. W. **A flat embedding method for transmission electron microscopy reveals an unknown mechanism of tetracycline** (Communications biology, 8 Mar 2021)[https://doi.org/10.1038/s42003-021-01809-8]

Oberdorf, K., Hanft, A., Ramler, J., Krummenacher, I., Bickelhaupt, F. M., Poater, J., Lichtenberg, C. **Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radical-Coupling Reactions (Pn=N, P, As)The controlled release of well-defined radical species under mild conditions for subsequent use in selective reactions is an important and challenging task in synthetic chemistry. We show here that simple bismuth amide species [Bi(NAr2)3] readily release aminyl radicals [NAr2]. at ambient temperature in solution. These reactions yield the corresponding hydrazines, Ar2N−NAr2, as a result of highly selective N−N coupling. The exploitation of facile homolytic Bi−Pn bond cleavage for Pn−Pn bond formation was extended to higher homologues of the pnictogens (Pn=N–As): homoleptic bismuth amides mediate the highly selective dehydrocoupling of HPn** (Angewandte Chemie - International Edition, 15 Mar 2021)[https://doi.org/10.1002/anie.202015514]

Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M., Fernández, I. **Bifunctional Hydrogen Bond Donor-Catalyzed Diels–Alder Reactions: Origin of Stereoselectivity and Rate Enhancement** (Chemistry - A European Journal, 17 Mar 2021)[https://doi.org/10.1002/chem.202004496]

Lamoree, M., Hamers, T., Meijer, J., Antignac, J. P., Hutinet, S., Debrauwer, L., Covaci, A., Huber, C., von Krauss, M. K., Walker, D. I., Walker, D. I., Schymanski, E. L., Vermeulen, R., Vlaanderen, J. **An annotation database for chemicals of emerging concern in exposome research: Environmental exposures are a key contributor to disease and premature death (Landrigan et al., 2018). Yet, only a fraction of chemicals produced in significant amounts with potential to enter the environment have sufficient information to characterize human exposure levels and toxicity.Chemicals of Emerging Concern (CECs) include a very wide group of chemicals that are suspected to be responsible for adverse effects on health, but for which very limited information is available.General information** (Elsevier, 24 Mar 2021)[https://doi.org/10.1016/j.envint.2021.106511]

Hamlin, T. A., Bickelhaupt, F. M., Fernández, I. **The Pauli Repulsion-Lowering Concept in Catalysis** (Accounts of Chemical Research, 24 Mar 2021)[https://doi.org/10.1021/acs.accounts.1c00016]

Kort, R., Schlösser, J., Vazquez, A. R., Atukunda, P., Muhoozi, G. K., Wacoo, A. P., Sybesma, W. F., Westerberg, A. C., Iversen, P. O., Schoen, E. D. **Model selection reveals the butyrate-producing gut bacterium Coprococcus eutactus as predictor for language development in three-year-old rural Ugandan children** (medRxiv, 25 Mar 2021)[https://doi.org/10.1101/2021.03.15.21253665]

Jian, J., Hammink, R., McKenzie, C. J., Bickelhaupt, F. M., Poater, J., Mecinović, J. **Do Sulfonamides Interact with Aromatic Rings?** (Chemistry - A European Journal, 26 Mar 2021)[https://doi.org/10.1002/chem.202004732]

Yu, S., Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M. **How Oriented External Electric Fields Modulate Reactivity** (Chemistry: A European Journal, 26 Mar 2021)[https://doi.org/10.1002/chem.202004906]

Ho, V. Q., Verboom, T., Rong, M. K., Habjan, E., Bitter, W., Speer, A. **Heterologous Expression of eth** (Antimicrobial agents and chemotherapy, Apr 2021)[https://doi.org/10.1128/AAC.01445-20]

Silva, D. R., Santos, L. A., Hamlin, T. A., Guerra, C. F., Freitas, M. P., Bickelhaupt, F. M. **The Gauche Effect in XCH 2 CH 2 X Revisited** (ChemPhysChem, 7 Apr 2021)[https://doi.org/10.1002/cphc.202100090]

Santos, L. A., Lubbe, S. C. C., Hamlin, T. A., Ramalho, T. C., Bickelhaupt, F. M. **A Quantitative Molecular Orbital Perspective of the Chalcogen Bond** (ChemistryOpen, 17 Apr 2021)[https://doi.org/10.1002/open.202000323]