# AIMMS publication report for: 2020-10-26

### New papers: 2020-9/10

Landa, I., Westbroek, H., Janssen, F., van Muijlwijk-Koezen, J. E., Meeter, M. **Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking** (Science & Education, 7 Aug 2020)[https://doi.org/https://doi.org/10.1007/s11191-020-00145-3]

Aguiar, M. (ed.), Braumann, C. (ed.), Kooi, B. (ed.), Pugliese, A. (ed.), Stollenwerk, N. (ed.) **Current Trends in Dynamical Systems in Biology and Natural Sciences** (None, 2020)[https://doi.org/10.1007/978-3-030-41120-6]

Vermeeren, P., Hamlin, T. A., Fernández, I., Bickelhaupt, F. M. **Origin of rate enhancement and asynchronicity in iminium catalyzed Diels-Alder reactions** (Chemical Science, 21 Aug 2020)[https://doi.org/10.1039/d0sc02901g]

Grossi, J., Musslimani, Z. H., Seidl, M., Gori-Giorgi, P. **Kohn-Sham equations with functionals from the strictly-correlated regime: Investigation with a spectral renormalization method** (Journal of Physics Condensed Matter, 11 Nov 2020)[https://doi.org/10.1088/1361-648X/abace2]

Drienovská, I., Gajdoš, M., Kindler, A., Takhtehchian, M., Darnhofer, B., Birner-Gruenberger, R., Dörr, M., Bornscheuer, U. T., Kourist, R. **Folding Assessment of Incorporation of Noncanonical Amino Acids Facilitates Expansion of Functional-Group Diversity for Enzyme Engineering** (Chemistry - A European Journal, 25 Sep 2020)[https://doi.org/10.1002/chem.202002077]

Romasanta, A. K., van der Sijde, P., van Muijlwijk-Koezen, J. E. **Innovation in pharmaceutical R&D: mapping the research landscape** (None, 10 Oct 2020)[https://doi.org/https://doi.org/10.1007/s11192-020-03707-y]

### New papers: 2020

Krahfuß, M. J., Nitsch, J., Bickelhaupt, F. M., Marder, T. B., Radius, U. **N-Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence** (Chemistry - A European Journal, 1 Sep 2020)[https://doi.org/10.1002/chem.202001062]

Yu, S., Vermeeren, P., van Dommelen, K., Bickelhaupt, F. M., Hamlin, T. A. **Understanding the 1,3-Dipolar Cycloadditions of Allenes** (Chemistry - A European Journal, 4 Sep 2020)[https://doi.org/10.1002/chem.202000857]

De Santis, M., Belpassi, L., Jacob, C. R., Severo Pereira Gomes, A., Tarantelli, F., Visscher, L., Storchi, L. **Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions** (Journal of chemical theory and computation, 8 Sep 2020)[https://doi.org/10.1021/acs.jctc.0c00603]

Buchholz, F., Theophilou, I., Giesbertz, K. J., Ruggenthaler, M., Rubio, A. **Light-Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics** (Journal of chemical theory and computation, 8 Sep 2020)[https://doi.org/10.1021/acs.jctc.0c00469]

Xie, C., Albulescu, L. O., Bittenbinder, M. A., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J. **Neutralizing effects of small molecule inhibitors and metal chelators on coagulopathic Viperinae snake venom toxins** (Biomedicines, Sep 2020)[https://doi.org/10.3390/BIOMEDICINES8090297]

van de Ven, H. C., Purmova, J., Groeneveld, G., Bos, T. S., Gargano, A. F., van der Wal, S., Mengerink, Y., Schoenmakers, P. J. **Living with breakthrough: Two-dimensional liquid-chromatography separations of a water-soluble synthetically grafted bio-polymer** (Separations, Sep 2020)[https://doi.org/10.3390/separations7030041]

Stasyuk, O. A., Solà, M., Swart, M., Fonseca Guerra, C., Krygowski, T. M., Szatylowicz, H. **Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs** (ChemPhysChem, 15 Sep 2020)[https://doi.org/10.1002/cphc.202000434]

Landa, I., Westbroek, H., Janssen, F., van Muijlwijk, J., Meeter, M. **Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking** (Science and Education, 1 Oct 2020)[https://doi.org/10.1007/s11191-020-00145-3]

Pípal, M., Legradi, J., Smutná, M., Kočí, T., Priebojová, J., Bláhová, L., Krauss, M., Hilscherová, K. **Neurobehavioral effects of cyanobacterial biomass field extracts on zebrafish embryos and potential role of retinoids** (Aquatic Toxicology, Nov 2020)[https://doi.org/10.1016/j.aquatox.2020.105613]

Fumagalli, A., Heuninck, J., Pizzoccaro, A., Moutin, E., Koenen, J., Séveno, M., Durroux, T., Junier, M. P., Schlecht-Louf, G., Bachelerie, F., Schütz, D., Stumm, R., Smit, M. J., Guérineau, N. C., Chaumont-Dubel, S., Marin, P. **The atypical chemokine receptor 3 interacts with Connexin 43 inhibiting astrocytic gap junctional intercellular communication** (Nature Communications, 1 Dec 2020)[https://doi.org/10.1038/s41467-020-18634-y]