# AIMMS publication report for: 2020-11-09

### New papers: 2020-10/11

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]

Dohnalová, K., Hapala, P., Kůsová, K., Infante, I. **Electronic Structure Engineering Achieved via Organic Ligands in Silicon Nanocrystals** (Chemistry of Materials, 11 Aug 2020)[https://doi.org/10.1021/acs.chemmater.0c00443]

Bugatti, K., Bruno, A., Arosio, D., Sartori, A., Curti, C., Augustijn, L., Zanardi, F., Battistini, L. **Shifting Towards αVβ6 Integrin Ligands Using Novel Aminoproline-Based Cyclic Peptidomimetics** (Chemistry - A European Journal, 21 Oct 2020)[https://doi.org/10.1002/chem.202002554]

Janssen, F., Westbroek, H., Landa, I., van der Ploeg, B., van Muijlwijk-Koezen, J. E. **Perspectives for Teaching About How Science Works** (None, 2020)[https://doi.org/10.1007/978-3-030-57239-6\_14]

Ayad, L. A., Dourou, A. M., Arhondakis, S., Pissis, S. P. **Iso** (Genome Biology and Evolution, Sep 2020)[https://doi.org/10.1093/gbe/evaa171]

Salvito, D., Fernandez, M., Jenner, K., Lyon, D. Y., de Knecht, J., Mayer, P., MacLeod, M., Eisenreich, K., Leonards, P., Cesnaitis, R., León-Paumen, M., Embry, M., Déglin, S. E. **Improving the Environmental Risk Assessment of Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials** (Environmental toxicology and chemistry, 1 Nov 2020)[https://doi.org/10.1002/etc.4846]

Gritsenko, O. V. **Comparative metathermodynamic description of thermal and correlation electron effects** (Physical Review A, 8 Sep 2020)[https://doi.org/10.1103/PhysRevA.102.032806]

Van Meer, R., Gritsenko, O., Chai, J. D. **Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description** (Physical Review A, 15 Sep 2020)[https://doi.org/10.1103/PhysRevA.102.032815]

Celeiro, M., Armada, D., Dagnac, T., de Boer, J., Llompart, M. **Hazardous compounds in recreational and urban recycled surfaces made from crumb rubber. Compliance with current regulation and future perspectives** (Science of the Total Environment, 10 Feb 2021)[https://doi.org/10.1016/j.scitotenv.2020.142566]

Jian, J., Poater, J., White, P. B., Mckenzie, C. J., Bickelhaupt, F. M., Mecinović, J. **Probing Halogen-πversus CH-πInteractions in Molecular Balance** (Organic letters, 29 Sep 2020)[https://doi.org/10.1021/acs.orglett.0c02773]

Steinberg, R., Origi, A., Natriashvili, A., Sarmah, P., Licheva, M., Walker, P. M., Kraft, C., High, S., Luirink, J., Shi, W. Q., Helmstädter, M., Ulbrich, M. H., Koch, H. G. **Posttranslational insertion of small membrane proteins by the bacterial signal recognition particle** (PloS Biology, 30 Sep 2020)[https://doi.org/10.1371/journal.pbio.3000874]

Nieuwland, C., Zaccaria, F., Fonseca Guerra, C. **Understanding alkali metal cation affinities of multi-layer guanine quadruplex DNATo gain better understanding of the stabilizing interactions between metal ions and DNA quadruplexes, dispersion-corrected density functional theory (DFT-D) based calculations were performed on double-, triple- and four-layer guanine tetrads interacting with alkali metal cations. All computations were performed in aqueous solution that mimics artificial supramolecular conditions where guanine bases assemble into stacked quartets as well as biological environments in which telomeric quadruplexes are formed. To facilitate the computations on these significant larger systems, optimization of the DFT description was performed first by evaluating the performance of partial reduced basis sets. Analysis of the stabilizing interactions between alkali cations and the DNA bases in double and triple-layer guanine quadruplex DNA reproduced the experimental affinity trend of the order Li+< Rb+ < Na+ < K+. The desolvation and the size of alkali metal cations are thought to be responsible for the order of affinity. Nevertheless, for the alkali metal cation species individually, the magnitude of the bond energy stays equal for binding as first, second or third cation in double, triple and four-layer guanine quadruplexes, respectively. This is the result of an interplay between a decreasingly stabilizing interaction energy and increasingly stabilizing solvation effects, along the consecutive binding events. This diminished interaction energy is the result of destabilizing electrostatic repulsion between the hosted alkali metal cations. This work emphasizes the stabilizing effect of aqueous solvent on large highly charged biomolecules.General information** (Physical chemistry chemical physics : PCCP, 30 Sep 2020)[https://doi.org/10.1039/d0cp03433a]

van Beek, L. F., Surmann, K., van den Berg van Saparoea, H. B., Houben, D., Jong, W. S., Hentschker, C., Ederveen, T. H., Mitsi, E., Ferreira, D. M., van Opzeeland, F., van der Gaast–de Jongh, C. E., Joosten, I., Völker, U., Schmidt, F., Luirink, J., Diavatopoulos, D. A., de Jonge, M. I. **Exploring metal availability in the natural niche of Streptococcus pneumoniae to discover potential vaccine antigens** (Virulence, 5 Oct 2020)[https://doi.org/10.1080/21505594.2020.1825908]

Marino, S. D., Gerolin, A. **An Optimal Transport Approach for the Schrödinger Bridge Problem and Convergence of Sinkhorn Algorithm** (Journal of Scientific Computing, 1 Nov 2020)[https://doi.org/10.1007/s10915-020-01325-7]

Adihou, H., Gopalakrishnan, R., Förster, T., Guéret, S. M., Gasper, R., Geschwindner, S., Carrillo García, C., Karatas, H., Pobbati, A. V., Vazquez‐Chantada, M., Davey, P., Wassvik, C. M., Pang, J. K. S., Soh, B. S., Hong, W., Chiarparin, E., Schade, D., Plowright, A. T., Valeur, E., Lemurell, M., Grossmann, T. N., Waldmann, H. **A protein tertiary structure mimetic modulator of the Hippo signalling pathway** (Nature Communications, 1 Nov 2020)[https://doi.org/10.1038/s41467-020-19224-8]

Grimmel, S. A., Teodoro, T. Q., Visscher, L. **Is it worthwhile to go beyond the local-density approximation in subsystem density functional theory?** (International Journal of Quantum Chemistry, 1 Nov 2020)[https://doi.org/10.1002/qua.26111]

### New papers: 2020

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]

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]