DOI: 10.1002/qua.26587

EDITORIAL

International Journal of Quantum Chemistry WILEY

Germany's Future in Theoretical and Computational Chemistry: a Special Issue Celebrating DEAL

This special issue on computational and theoretical chemistry highlights the work of early career researchers affiliated with German research institutions. It is intended to celebrate the DEAL agreement on open-access publishing between Wiley and more than 700 publicly funded German research organizations, collected in *Project DEAL* by the Rector's Conference on behalf of the Alliance of Science Organizations in Germany. Open-access publications enable all researchers to gain and share knowledge regardless of economic or geographic barriers and can hence be considered as one of the cornerstones of free science. Among the different models that are being tested at the moment, DEAL could represent one of the first steps toward general open-access publishing in science.

While the terms *young*, *emerging*, or *early career* have varying definitions, the focus in this collection lies on those who are pursuing independent lines of research but do not yet hold a permanent professorship. The 15 contributors to this issue obtained their doctoral degrees between 2010 and 2016. At the time of invitation, the authors held a variety of positions, including postdoctoral researchers pursuing their *venia legendi*, group leaders at various research institutions, independent fellowship holders, and (junior) professors with and without tenure track. This reflects the multitude of possible academic career paths in Germany, which have become available only in the past two decades.

Following the idea of Born and Oppenheimer, the contributions in this issue focus either on the description of electronic structure problems or deal with nuclear motion on potential energy surfaces. The former type of contribution includes a report by Kati Finzel[1] on an analytical approximation for the Pauli potential to be used during kinetic energy evaluations in orbital free density functional theory (DFT). Furthermore, Giovanni Bistoni and coworkers[2] evaluate the dependence of a local energy decomposition approach for domain-based pair natural orbital-coupled cluster theory (DLPNO-CC) on the basis set and on various technical parameters within the S66 set for non-covalent interactions. Giovanni Li Manni et al.[3] present an in-depth analysis of strong correlation effects in a ferrous porphyrin model based on a set of multireference calculations with large active spaces. Addressing similar iron environments, Vera Krewald and coworkers[4] present a calibration study for Mössbauer spectroscopy including an interactive, web-based notebook by Jonny Proppe for uncertainty estimates of DFT predictions.

The research article contributed by Benjamin Helmich-Paris[5] introduces an extension of their recently developed linear-response complete active space self-consistent field method to the calculation of X-ray absorption spectra. Alternative approaches to the computation and analysis of such spectra based on DFT and second-order perturbation theory were employed by Michael Roemelt and coworkers[6] in their work on the spectral properties of multiple copper porphyrazines. Róbert Izsák[7] provides a perspective on a similarity-transformed equation of motion DLPNO-CC approach for the calculation of electronically excited states, and compares its results against experimental absorption band maxima of BODIPY dyes.

In the Born–Oppenheimer picture, the electronic structure gives rise to adiabatic potential energy surfaces on which the nuclei move. With pysisyphus, Stephan Kupfer, together with Johannes Steinmetzer and Stefanie Gräfe[8], presents a software to find stationary points and reaction paths on ground and excited state potential energy surfaces. That these stationary points can be altered by an environment is shown by Mariana Rossi and coworkers[9], who present a first-principles database that allows to clarify the effect of different metal surfaces on the conformational space of a flexible amino acid, finding stereoselective binding in some cases. When environments represent a large part of the full system, accurate results can also be obtained by multi-level or fragmentation-based schemes. Sebastian Höfener[10] reports on the KOALA software package, which focuses on the combination of different quantum-mechanical methods with the fragments interacting by orbital-free DFT with a special attention to response properties. The perspective by Tim Stauch[11] reviews different approaches to model molecules and reactions under pressure, outlining the current challenges in treating this different environmental aspect.

The possibility to explore potential energy surfaces in a variety of environments naturally leads to the study of nuclear dynamics. In a perspective, Carolin König[12] discusses multi-level approaches for the accurate calculation of relevant features in anharmonic vibrational spectra with vibrational wave functions. Adrien Marjollet and Ralph Welsch[13] benchmark a method that combines quasi-classical trajectories and ring polymer molecular dynamics to obtain state-selective cross sections of bimolecular reactions, approximately including nuclear quantum effects. However, a full quantum treatment of electrons and nuclei is not always necessary and techniques like QM/MM or full MM can be employed. For example, Götze et al.[14] present a new QM/MM software interface (gmx2qmmm), that offers novel ways to treat the QM/MM boundary region, showing how it fares for flexible amino-acid conformations and the calculation of UV/vis spectra. Finally, Oldamur Hollóczki[15] investigates the stability of oligoalanines in the presence of plastic nanoparticles through simulated annealing and semi-empirical approaches for the conformational search and stability assessment, respectively.

https://doi.org/10.1002/qua.26587

Naturally, this special issue showcases only a fraction of the scientific generation that was influenced by the diversification of research opportunities for early career scientists. In view of the above-mentioned contributions, we can confidently note that the variety of methods, the breadth of topics, the detail of study, and the scope of application areas demonstrate the creativity and productivity of early career researchers in independent settings.

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