Application of *GW*-BSE theory to transition-metal complexes

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The Bethe-Salpeter equation (BSE) was initially derived in nuclear physics and later imported to the field of computational solid-state physics. Recently, it has been widespread for calculating molecular excitation energies and provided optimistic results in a variety of systems. The BSE formalism is very similar to the time-dependent density functional theory (TDDFT) in the language of linear response, and thus has the same scaling with respect to system size as TDDFT. However, BSE can be applied for description of excitations that are particularly problematic for TDDFT, e.g. excitations with charge-transfer character. The BSE approach has recently been implemented in our TURBOMOLE program using a resolution-of-the-identity (RI) approximation for all two-electron integrals that are required to solve the equation. Since BSE normally requires quasiparticle energies from preceding *GW* calculations as input, *GW* and BSE have often emerged together, which is known as the *GW*-BSE formalism. The performance of the BSE approach for the computation of singlet and triplet excitation energies of small molecules has been assessed with respect to the quasiparticle energies used in the BSE calculations. Here we present several examples of application of *GW*-BSE to transition-metal complexes.

References
1. K. Krause, W. Klopper, *J. Comput. Chem.* **38** (2017), 383.
2. D. Jacquemin, I. Duchemin, X. Blase, *J. Phys. Chem. Lett.* **8** (2017), 1524.
3. X. Gui, C. Holzer, W. Klopper, *J. Chem. Theory Comput.* **14** (2018), 2127.
4. S. V. Kruppa, C. Groß, X. Gui, et al. *Chem. Eur. J.* 10.1002/chem.201901981.