# Recent advances in describing dispersion / van der Waals interactions

**Christof Holzer**[1], **Wim Klopper**[1]

[1]*Institut für Physikalische Chemie, Karlsruher Institut für Technologie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany*

We aim at developing new variants and methods to improve predictions on binding energies of van der Waals bonded systems. A main working tool for this task is the symmetry-adapted perturbation theory ("SAPT") that has been newly implemented into our working package TURBOMOLE. To improve on existing theory, we enhanced certain aspects of SAPT:

1) Our main goal is to use explicitly correlated functions which help improve the basis set convergence. The dispersion energy is a correlation energy and therefore suffers from slow basis set convergence. We therefore aim at employing the F12 methodology to improve basis set convergence. First tests have shown that the convergence can be improved by up to two cardinal numbers compared to standard basis sets. [1]
2) Heavy elements constitute a challenge for quantum chemical methods. To further investigate the nature of e.g. metal – π or aurophilic interactions we implemented a two-component version of DFT-SAPT into Turbomole.
3) With a combined $G_0W_0$-BSE-SAPT approach we aim at minimizing the influence of the DFT XC kernel on the energy components of the SAPT scheme.

[1] J. A. Frey, C. Holzer, W. Klopper, and Samuel Leutwyler, Chem. Rev., 116, 5614 (2016)