# Local correlation methods for molecular properties

Martin Schütz[1]

[1] *Institute of Physical and Theoretical Chemistry, University of Regensburg, Universitätsstraße 31, D-93040 Regensburg, Germany*

Presently, efficient local correlation methods for calculating molecular properties are available in MOLPRO. These include excitation energies, corresponding transition strengths, and first-order properties (like dipole moments) of ground and excited states [1–5]. Furthermore, recently, also nuclear magnetic shielding tensors in the GIAO framework have been implemented at the level of the local MP2 method.

In my contribution I will give a report on these recent advances and present some illustrative applications.

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[1] D. Kats, T. Korona, and M. Schütz *J. Chem. Phys.*, vol. 125, p. 104106, 2006.
[2] D. Kats, T. Korona, and M. Schütz *J. Chem. Phys.*, vol. 127, p. 064107, 2007.
[3] D. Kats and M. Schütz *J. Chem. Phys.*, vol. 131, no. 12, p. 124117, 2009.
[4] D. Kats and M. Schütz *Z. Phys. Chem.*, vol. 224, pp. 601–616, 2010.
[5] K. Freundorfer, D. Kats, T. Korona, and M. Schütz *J. Chem. Phys.*, vol. 133, p. 244110, 2010.