A Quantum Leap Into the Future of Chemistry

# What's New in Q-Chem

Feature 10

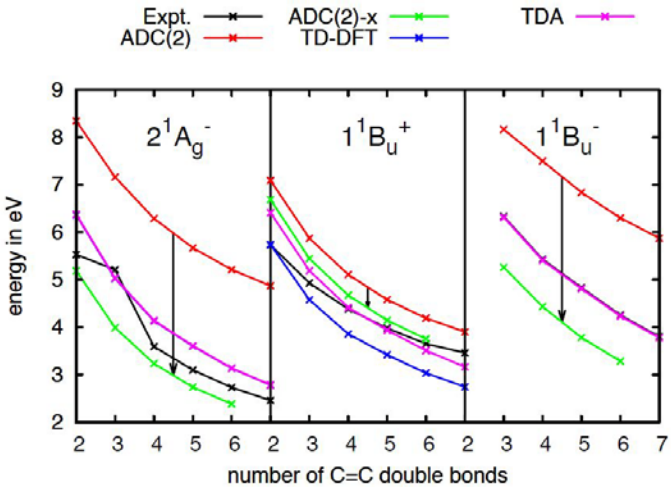
## Correlated Excited States with the Algebraic Diagrammatic Construction (ADC) Scheme

**Developers:** Michael Wormit, Andreas Dreuw

The reliable calculation of excited states of larger molecules is essential for the theoretical understanding of photo-induced processes. We have implemented the Algebraic Diagrammatic Construction (ADC) scheme up to second order in perturbation theory allowing for the computation of vertical excited states and their transition moments.

The ADC scheme represents an alternative excited state method to the more common CI and CC approaches. It has the advantage of being size-consistent and more compact, while retaining hermiticity. This feature should be used for the calculation of excited states with single and double excitation character

The graph shows the dependence of the vertical excitation energies of the three lowest excited states of linear polyenes on the number of conjugated double bonds. The comparison of the excitation energies obtained with strict and extended ADC(2) provides a useful diagnostic for the importance of double excitations in the theoretical description of the excited states. In this case the energies of the doubly excited $A_g^-$ and $B_u^-$ states drop significantly while the singly excited $B_u^+$ state is mostly unaffected.




For more new features, visit:
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## Correlated Excited States with the Algebraic Diagrammatic Construction (ADC) Scheme (continued)


Andreas Dreuw Michael Wormit

Publications: J. Starcke, M. Wormit, J. Schirmer, A. Dreuw, "How much double excitation character do the lowest excited states of linear polyenes have? " Chem. Phys. 239, 39 (2006)

S. Knippenberg; J. Starcke; M. Wormit; A. Dreuw, "The low-lying excited states of neutral polyacenes and their radical cations: a quantum chemical study employing the algebraic diagrammatic construction scheme of second order ." Mol. Phys. 108, 2801 (2010)

For more information on how to use this feature, refer to the Q-Chem Manual, Section 6.7.

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