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 - The original DFT/MRCI program: A combination of Kohn–Sham density functional theory and multi-reference configuration interaction methods. S. Grimme and M. Waletzke, *J. Chem. Phys.* 111, 5645 (1999)
 - The parallel version: Parallel multireference configuration interaction calculations on mini- β -carotenes and β -carotene. Martin Kleinschmidt, Christel M. Marian, Mirko Waletzke and Stefan Grimme *J. Chem. Phys.*, 130, 044708[1-11] (2009) DOI: 10.1063/1.3062842
 - The R2016 Hamiltonian: Redesign of the DFT/MRCI Hamiltonian. Igor Lyskov, Martin Kleinschmidt and Christel M. Marian *J. Chem. Phys.*, 144, 034104 (2016) DOI: 10.1063/1.4940036
 - The R2017 Hamiltonian: DFT/MRCI Hamiltonian for odd and even numbers of electrons. Adrian Heil and Christel M. Marian *J. Chem. Phys.*, 147, 194104 (2017) DOI: 10.1063/1.5003246
 - The R2018 Hamiltonian: On the performance of DFT/MRCI Hamiltonians for electronic excitations in transition metal complexes: The role of the damping function. Adrian Heil, Martin Kleinschmidt and Christel M. Marian *J. Chem. Phys.*, in press (2018)
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