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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- $\beta$ -carotenes and  $\beta$ -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.*, 149, 164106 (2018) DOI: 10.1063/1.5050476
  - The R2022 Hamiltonian: R2022: A DFT/MRCI ansatz with improved performance for double excitations. Dennis Dombrowski, Timo Schulz, Martin Kleinschmidt and Christel M. Marian *J. Phys. Chem. A*, 127, 2011-2025 (2023) DOI: 10.1021/acs.jpca.2c07951
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