

PARAMETRIZATION OF THE SECOND-ORDER REDUCED DENSITY MATRIX IN REDUCED DENSITY MATRIX FUNCTIONAL THEORY

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Why even bother with Reduced Density Matrix (RDM)?

RDM vs wavefunction

Objectives of the work

Definition of RDMs

Foundation of RDMFT

LS approximation

BBC approximation

A POSSIBLE NEW PARAMETRIZATION

Our 2-RDM

Optimization of the 2-RDM

Energy computation

Minkowski distances

Energy results & errors

Minkowski distance results

Conclusions