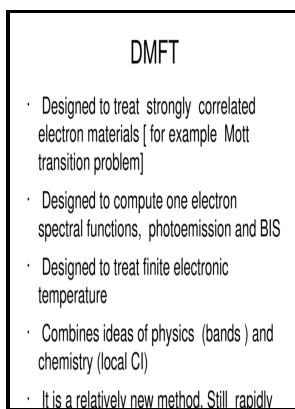


# Electronic structure of molecules - a new approach

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Notes: Bibliography: p. 161-162.  
This edition was published in 1964



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## New Methods For Electronic Structure Calculations on Large Molecules, Annual Review of Physical Chemistry

In the current work, we explore a MIM scheme which first partitions a molecule into nonoverlapping fragments and then recombines the interacting fragments to form overlapping subsystems. {Mn14W48} aggregate: the perspective of isopolyanions as ligands.

## The electronic structure of molecules: a new approach, (Book, 1964) [tech.radiozamaneh.com]

Analysis of the Errors in the Electrostatically Embedded Many-Body Expansion of the Energy and the Correlation Energy for Zn and Cd Coordination Complexes with Five and Six Ligands and Use of the Analysis to Develop a Generally Successful Fragmentation Strategy. The approach presented in this monograph goes back to the fundamentals in that it is exclusively based on interactions involving nuclear and electronic charges. ACS Chemical Biology 2013, 8 11 , 2354-2359.

## Novel computational approach launches new paradigm in electronic structure theory

Effective Fragment Potential Method: Past, Present, and Future.

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Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides.

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Dalton Transactions 2012, 41 37 , 11402. Two New Sandwich-Type Manganese {Mn5}-Substituted Polyoxotungstates: Syntheses, Crystal



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