

Electronic structure of molecules - a new approach

Methuen - Molecules



Description: -

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Quine, W. V.

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Notes: Bibliography: p. 161-162.

This edition was published in 1964



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Charge Distributions and Chemical Effects

Accounts of Chemical Research 2014, 47 9 , 2731-2738. The Journal of Physical Chemistry Letters 2019, 10 24 , 7836-7841.

Charge Distributions and Chemical Effects

Extrapolation to the Gold-Standard in Quantum Chemistry: Computationally Efficient and Accurate CCSD T Energies for Large Molecules Using an Automated Thermochemical Hierarchy. Emiliano Deustua and senior postdoctoral associate Jun Shen. Journal of Chemical Theory and Computation 2013, 9 2 , 1036-1042.

Novel computational approach launches new paradigm in electronic structure theory

Journal of Chemical Theory and Computation 2019, 15 7 , 3991-4002.

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This analysis allows electronic excitations to be described by building upon ground state electronic structures, without the need for molecular orbitals. Nanoscale 2013, 5 24 , 12565. The many-particle Schrödinger is at the heart of the problem.

Electronic transitions of molecules: vibrating Lewis structures

The Journal of Physical Chemistry Letters 2017, 8 14 , 3415-3420. Since the charge density describes the distribution of negative charge in real space, it is a physically measurable quantity. A new approach to the deposition of Mn 12 single-molecule magnet monolayers on the functionalized Au 111 surface optimized for the investigation by means of scanning tunneling spectroscopy was developed.

The electronic structure of molecules: a new approach, (Book, 1964) [metrics.learnindialearn.in]

Journal of Chemical Theory and Computation 2018, 14 6 , 2852-2866. Chemical Reviews 2015, 115 12 , 5607-5642. In this method, we use a multilevel partitioning approach coupled with electronic structure studies at multiple levels of theory to provide a hierarchical strategy for

systematically improving the computed results.

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