## Advances In The Theory Of Quantum Systems In Chemistry And Physics

## **DOWNLOAD HERE**

From the contents: Time Asymmetry and the Evolution of Physical Laws.- Spatially-Dependent-Mass Schrdinger Equations with Morse Oscillator Eigenvalues: Isospectral Potentials and Factorization Operators.- Relativistic Theory of Cooperative Muon-Nuclear Processes: Negative Muon Capture and Metastable Nucleus Discharge.- Two-Range Addition Theorem for Coulomb Sturmians.- Why Specific ETOs are Advantageous for NMR and Molecular Interactions.- Progress in Hylleraas-CI Calculations on Boron.- Structural and Electronic Properties of Polonium under Hydrostatic Pressure.- Complexity Analysis of the Hydrogenic Spectrum in Strong Fields.- Atomic Density Functions: Atomic Physics Calculations Analyzed with Methods from Quantum Chemistry.- Understanding Maximum Probability Domains with Simple Models.- Density Scaling for Excited States.- Finite Element Method in DFT Electronic Structure Calculations.- Shifts in Excitation Energies Induced by Hydrogen Bonding: A Comparison of the Embedding and Supermolecular Time-Dependent DFT Calculations with the Equation-of-Motion Coupled-Cluster Results.- Multiparticle Distribution of Fermi Gas System in Any Dimension.- Hierarchical Effective-Mode Approach for Extended Molecular Systems.- Short-Time Dynamics through Conical Intersections in Macro-systems: Quadratic Coupling Extension.- Theoretical Methods for Nonadiabatic Dynamics on the fly in Complex Systems and its Control by Laser Fields.- A Survey on Reptation Quantum Monte Carlo.- Quantum Monte Carlo Calculations of Electronic Excitation Energies: the Case of the Singlet n (CO) Transition in Acrolein.- Analysis of the Charge-Transfer Mechanism in Ion-Molecule Collisions.- Recombination by Electron Capture in the Interstellar Medium.-Systematic Exploration of Chemical Structures and Reaction Pathways on the Quantum Chemical Potential Energy Surface by Means of the Anharmonic Downward Distortion-Following Method.- Neutral Hydrolysis of Methyl Formate from Ab-initio Potentials and Molecular Dynamics Simulation.- Radial Coupling and Adiabatic Correction for the LiRb Molecule.- Centre-of-Mass Separation in Quantum Mechanics: Implications for the Many-Body Treatment in Quantum Chemistry and Solid-State Physics.-Anti-Adiabatic State - Ground Electronic State of Superconductors.- Delocalization Effects in Pristine and Oxidized Graphene Substrates.- A Review of Bonding in Dendrimers and Nano-Tubes.- 20-Nanogold Td and Low-Energy Hollow Cages: Void Reactivity.- A Theoretical Study of Complexes of Crown Ethers with Substituted Ammonium Cations.- Systematic Derivation and Testing of AMBER Force Field Parameters for Fatty Ethers from Quantum Mechanical Calculations.- Theoretical Studies on Metal-Containing Artificial DNA Bases. EAN/ISBN: 9789400720763 Publisher(s): Springer, Berlin, Springer Netherlands Discussed keywords: Quantenphysik Format: ePub/PDF Author(s): Hoggan, Philip E. - Brndas, Erkki J. - Maruani, Jean

## **DOWNLOAD HERE**

Similar manuals: