DV-X a Molecular Orbital Calculation Method

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This book describes the basic aspects of molecular orbital calculations based on quantum mechanics, including both time-independent and time-dependent formalisms, and explains how to calculate an electric dipole transition and an electronic structure under an electric field. The authors discuss basic quantum mechanics, explain how to modify the basic quantum mechanical equations for use in computer calculations, and provide numerical examples of calculations that can be performed easily using programs such as Excel(TM). This unique text will be of interest to professionals and students in many fields including quantum science and chemistry, mathematics, computer programming, and engineering.

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