



Valence Bond Methods: Theory and Applications

Gordon A. Gallup

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Valence bond theory is one of two commonly used methods in molecular quantum mechanics, the other is molecular orbital theory. This book focuses on the first of these methods, ab initio valence bond theory. The book is split into two parts. Part I gives simple examples of two-electron calculations and the necessary theory to extend these to larger systems. Part II gives a set of case studies of related molecule sets designed to show the nature of the valence bond description of molecular structure. It also highlights the stability of this description to varying basis sets. There are references to the CRUNCH computer program for molecular structure calculations which is currently available in the public domain. The book will be of primary interest to researchers and students working on electronic theory and computation in chemistry and chemical physics.

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