

Valence Bond Theory (Theoretical and Computational Chemistry)

David Cooper

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Valence bond (VB) theory, which builds the descriptions of molecules from those of its constituent parts, provided the first successful quantum mechanical treatments of chemical bonding. Its language and concepts permeate much of chemistry, at all levels. Various modern formulations of VB theory represent serious tools for quantum chemical studies of molecular electronic structure and reactivity. In physics, there is much VBbased work (particularly in semi-empirical form) on larger systems.

Importance of Topic

The last decade has seen significant advances in methodology and a vast increase in the range of applications, with many new researchers entering the field.

Why This Title

Valence Bond Theory succeeds in presenting a comprehensive selection of contributions from leading valence bond (VB) theory researchers throughout the world. It focuses on the vast increase in the range of applications of methodology based on VB theory during the last decade and especially emphasizes recent advances.



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