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1 Introduction ; 2 Spin States in Bimetallic Clusters: Effects on Structure and Energetics
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References
A Hybrid Functional for the Exchange-Correlation Kernel in Time-Dependent Density Functional Theory

Sommario/riassunto

In the last few years, much attention has been given by theoretical chemists to the development of more accurate model functionals and faster computational techniques including excited electronic states. The 8th International Conference on the Applications of Density Functional Theory to Chemistry and Physics, held in Rome, Italy, on 6-10 September 1999, gathered chemists and physicists to present and discuss state-of-the-art methodological developments and applications of density functional theory (DFT) to increasingly complex systems. The scientists shared their knowledge and experience in