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Atomistic Modeling of Condensed-Phase ReactionsFirst Principles Simulations of High Explosives; Conclusions; Acknowledgments; References; 5. Magnetic Properties of Atomic Clusters of the Transition Elements; Introduction; Basic Concepts; Experimental Studies of the Dependence of the Magnetic Moments with Cluster Size; Simple Explanation of the Decay of the Magnetic Moments with Cluster Size; Tight Binding Method; Tight Binding Approximation for the d Electrons; Introduction of s and p Electrons; Formulation of the Tight Binding Method in the Notation of Second Quantization
Spin-Density Functional TheoryGeneral Density Functional Theory; Spin Polarization in Density Functional Theory; Local Spin-Density Approximation (LSDA); Noncollinear Spin Density Functional Theory; Measurement and Interpretation of the Magnetic Moments of Nickel Clusters; Interpretation Using Tight Binding Calculations; Influence of the s Electrons; Density Functional Calculations for Small Nickel Clusters; Orbital Polarization; Clusters of Other 3d Elements; Chromium and Iron Clusters; Manganese Clusters; Clusters of the 4d Elements; Rhodium Clusters; Ruthenium and Palladium Clusters
Effect of Adsorbed Molecules

Sommario/riassunto

VOLUME 25Reviews in Computational ChemistryKenny B. Lipkowitz and Thomas R. CundariThis Volume, Like Those Prior To It, Features Pedagogically Driven Reviews By Experts In Various Fields Of Computational Chemistry. Volume 25 Contains: Eight Chapters Covering The Glass Transition In Polymer Melts, Atomistic Modeling Of Friction, The Computation Of Free Volume, Structural Order And Entropy Of Liquids And Glasses, The Reactivity Of Materials At Extreme Conditions, Magnetic Properties Of Transition Metal Clusters, Multiconfigurational Quantum Methods For The Treatment Of He