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Titolo	Modification of Magnetic Properties of Iron Clusters by Doping and Adsorption : From a Few Atoms to Nanoclusters / / by Gennady L. Gutsev, Kalayu G. Belay, Lavrenty G. Gutsev, Charles A. Weatherford
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Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Introduction -- Peculiarities of the Fe – Fe bonding -- Oxides and superhalogens with a single Fe center -- Interactions of small iron clusters with C and O atoms -- Interactions of small iron clusters with OH, NO, CO, and H2O -- Structure and magnetic properties of larger neutral and charged iron clusters -- Anomalous total spin magnetic moment of Fe EQ \O(13,+) -- Doping of icosahedral Fe13 with 3d- and 4d-atoms -- Doping of iron clusters with a Gd atom -- Iron oxide isomers of (FeO)12 and superexchange mechanism in (FeO)2 -- Interaction of iron clusters with carbon atoms and carbon monoxide -- Summary.
Sommario/riassunto	This brief is based on computations performed on unary neutral and charged iron clusters, binary iron clusters, and iron clusters interacting with carbon and oxygen atoms as well as with a number of diatomics and water. The author considers geometrical structure, thermodynamic

stability and electronic properties which are compared with experimental data. Special attention is paid to the dependence of total spin magnetic moments of iron clusters on their size, charge and interactions with dopant and absorbed atoms. In the dopant case, species such as 3d-metal, 4d-metal, Al, and Gd atoms are considered. In the adsorption case interactions of carbon atoms with iron clusters as the initial stage of catalyzed carbon nanotube growth are presented. Interactions of iron clusters with oxygen atoms are presented and the superexchange mechanism is discussed. Of special interest is the tracking of changes due to the evolution from a few atoms to a nanocluster.