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New Theoretical Aspects Topics In Current Chemistry

J Elliott



New Theoretical Aspects Topics In Current Chemistry:

Chemistry and Physics of Solid Surfaces V R. Vanselow, R. Howe, 2013-11-21 This volume contains review articles which were written by the invited speakers of the Sixth International Summer Institute in Surface Science ISSS held at the University of Wisconsin Milwaukee in August 1983 The objective of ISSS is to bring together a group of internationally recognized experts on various aspects of surface science to present tutorial review lectures over a period of one week Each speaker is asked in addition to write a review paper on his lecture topic The collected articles from previous Institutes have been published under the following titles Surface Science Recent Progress and Perspectives Crit Rev Solid State Sci 4 124 559 1974 Chemistry and Physics of Solid Surfaces Vol I 1976 Vol II 1979 Vol III 1982 CRC Press Boca Raton FL and Vol IV 1982 Springer Ser Chern Phys Vol 20 Springer Verlag Berlin Heidelberg New York 1982 No single collection of reviews or one week conference for that matter can possibly cover the entire field of modern surface science from heterogeneous catalysis through semiconductor surface physics to metallurgy It is intended however that the series Chemistry and Physics of Solid Surfaces as a whole should provide experts and students alike with a comprehensive set of reviews and literature references on as many aspects of the subject as possible particular emphasis being placed on the gas solid interface Each volume is introduced with a historical review of the development of one aspect of surface science by a distinguished participant in that development

High Resolution NMR Spectroscopy in Solids M. Mehring, 2012-12-06 Manipulation and Dilution Tools for Ruling Abundant Species NMR is dead was the slogan heard in the late 1960s at least among physicists until John S Waugh and his co workers initiated a series of new NMR experiments which employed the coherent modulation of interactions by strong radiofrequency fields A wealth of new phenomena was observed which are summarized in the introduction for the convenience of the unbiased reader whereas Section 2 collects the basic spin interactions observed in solids Line narrowing effects in dipolar coupled solids by the application of multiple pulse experiments are extensively discussed in Section 3 Numerous extensions of the basic Waugh Huber and Haeberlen experiment have been developed by different groups and have been applied to the nuclei ^1H ^9Be ^{19}F ^{27}Al ^{31}P ^{63}Cu in solids Application of this technique to a variety of systems is still in progress and should reveal interesting insights into weak spin interactions in solids It was soon realized that rare spins could be used as monitors for molecular fields in the solid state however rare spin observation is difficult because of the small signal to noise ratio Pines Gibby and Waugh introduced a new concept of cross polarization based on ideas of Hahn and co workers which allows the detection of rare spins with increased sensitivity The dynamics involved are treated in detail Other sections merely list results obtained by the techniques described and demonstrate their usefulness in the investigation of dynamical problems in molecular and solid state physics

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the Evaluation of Electronic Energy Matrix Elements Jürgen Hinze,1981-02 During the last thirty years with the
 development of high speed electronic computers methods have evolved which permit an accurate and quantitative ab initio
 determination of the electronic wavefunctions of atoms and molecules Thus a detailed elucidation of the electronic energy
 and structure of molecules has become possible using quantum mechanics directly However it is necessary if such
 calculations are to yield accurate and reliable results to include electron correlation explicitly which requires in general
 configuration mixing procedures with an extremely large number of configurations of the order of 10 configurations With
 eigenvalue problems of this size the limits of even the largest and fastest computers are reached rapidly and their solution
 has become possible only because direct methods have been developed which permit the determination of eigenvalues and
 eigenvectors for such large matrices iteratively without constructing the energy matrix explicitly These direct methods had
 been limited to the description of closed shell systems i.e systems with a single dominant closed shell reference determinant
 This limitation arose because with an open shell reference or with several reference determinants no procedures were known
 which allowed a rapid calculation of the energy matrix elements between configurations with general and widely different
 spin couplings which would be necessary Recently such methods have been developed based on early work of Gelfand
 Biedenharn and Moshinski using a unitary group representation of different spin coupled states Paldus achieved an
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