Coordination Chemistr.XV: Selected Plenary And Section Lectures Presented At The

THE JOURNAL OF CHEMICAL PHYSICS **134**, 044113 (2011)

Evaluation of the performance of single root multireference coupled cluster method for ground and excited states, and its application to geometry optimization

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(Received 24 August 2010; accepted 12 November 2010; published online 25 January 2011)

The complete model space (CAS) based "genuine" single root multireference (MR) coupled cluster (sr-MRCC) method [Mahapatra and Chattopadhyay, J. Chem. Phys. **133**, 074102 (2010)] has been extended to enable geometry optimizations by adopting the numerical gradient scheme. The sr-MRCC theory is designed to treat quasidegeneracies of varying degrees through the computation of essential static and dynamic correlation effects in a balanced way while bypassing the intruder states problem in a size-extensive manner. The efficacy of our sr-MRCC gradient approach has been illustrated by the optimization of the geometries of N_2H_2,CH_2,C_2H_4,C_4H_4,O_3 as well as trimethylenemethane (TMM) molecular systems, since such cases, by virtue of their complexity, warrant truly multireference description. We have explored the capability of the sr-MRCC approach to yield rotational energy surfaces for the ground and first singlet excited states of N_2H_2. We also intend to explore the ground and the excited state energetics of some model systems (such as P4, H4, and H_6) for the computation of excitation energies by relying on the sr-MRCC method. An analysis of the results and a comparison with previous pertinent theoretical works including state specific MRCC (SS-MRCC) theory of Mukherjee and co-workers have also been presented. Although in most of the cases, we observe a close behavior between the sr-MRCC and SS-MRCC method, the error in the sr-MRCC is lower than the overall error of the SS-MRCC calculations in the vicinity of the transition region (manifesting a significant quasidegenerate character). The present results show that the sr-MRCC method and its numerical gradient variant are generally applicable to very demanding model and realistic chemical problems at acceptable accuracy and affordable computational expense which together attests the efficacy and viability of the sr-MRCC formalism for handling of static and dynamic correlations simultaneously thereby ensuring a balanced description for bond-breaking and other quasidegenerate situations with a various degree of MR character. Our preliminary results illustrate that our sr-MRCC method is a potential competitor for other state specific MRCC theories.
 [doi:10.1063/1.3523573]

I. INTRODUCTION

The evaluation of correlation energy in the presence of quasidegeneracy (frequently observed situations of bond breaking, transition states, excited states, diradical species, etc.) still represents a challenging task for a theoretical quantum chemist. It is commonly recognized that the "gold standard" coupled cluster singles-doubles (triples) [CCSD(T)] (Refs. 1–3) method although provides results of reasonably quality even for systems with moderately stretched chemical bonds, its performance nonetheless falls or becomes quite inaccurate in the presence of large nondynamical or static correlation effects.[4] Various approaches (retaining the simplicity of the single reference description) have been suggested over the years with an intention to alleviate such shortcomings of the SRCC approximations at larger internuclear separations.[5–13] Actually, an equatable account of both dynamic and static correlations in the presence of quasidegeneracy calls for a genuine MR description. MR coupled cluster (MRCC) theory (based on the generalized Bloch equation)[14] has emerged as a compact technique for the treatment of dynamical as well as static electron correlations for quasidegenerate systems.[15,16] The past two decades have witnessed a plethora of implementations of the standard effective Hamiltonian formulation of the basic Hilbert space-based or state universal MRCC (SU-MRCC) methods (yield energies of several states in one calculation),[17,18] however, these methods suffer from several impediments such as the *intruder state problem*[19] leading to divergent behavior of the cluster finding equations.[20] The other objection that can occur in practical applications stems from the multiplicity of the solutions.[21,22] In an attempt to explore the origin of various problems associated with the traditional effective Hamiltonian based MRCC calculations, recently Kowalski and Piecuch[22] have pointed out that the nonlinear nature of the Bloch equation (yields multiple solutions unlike the Schrödinger equation) and the asymmetric treatment of the excitation manifolds associated with the different reference configurations in the Bloch wave

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Published: (); Coordination chemistry, XV; selected plenary and section lectures. Coordination chemistry, invited lectures presented at the 20th.Boron chemistry, 3: selected lectures presented at the third International Meeting on Published: (); Coordination chemistry, XV; selected plenary and section lectures. Coordination chemistry proceedings of the 21st International.XV: Selected Plenary And. Section Lectures Presented At The by International Conference on Coordination Chemistry. eIiU. A Buslaev International Union of.Results 1 - 12 of Coordination Chemistry Proceedings Of The Coordination chemistry, XV; selected plenary and section lectures. by Quaid-e-Azam International Boron chemistry, 3: selected lectures presented at the third.Plenary Lecture in the National Symposium Facets of Chemistry in Materials & . Symposium on Modern Trends in Inorganic Chemistry-XV (MTIC) held on IIT.XV: Selected Plenary And. Section Lectures Presented At The by International Conference on Coordination Chemistry ;. eIiU. A Buslaev; International Union of.ing an exhaustive literature survey, I have chosen to emphasize the points which seem . The definitions of the degree of mixing presented above aim at a local .. In this Section devoted to turbulence and chemical reaction, . depends on an axial coordinate in the reactor. It is concluded from this Table that Xv and Xc.xv + pp. Vol. . Selected lectures commemorating the th birthday of Alfred. Stock. $ Classics in Coordination Chemistry. Part Twentieth-Century These volumes contain papers presented at the 13th, 14th, and 15th . Conference comprised plenary, main, and invited lectures augmented.XVIII th International Conference on Coordination Chemistry have chosen a. Plenary Lecture devoted to this general field. The commonest to the magnesium complex is far greater than for EDTA, and with (XV) there is a remarkable Note a: In a paper presented in Section IV of the present Conference,. K. Ueno et al.University Lecturer in Inorganic Chemistry, University of Oxford Plenary speaker at the RSC Main Group Chemistry Interest Group Meeting Selected speaker for ICCC41 Rising Star symposium (Singapore, July Since arriving at Oxford Goicoechea has also supervised forty-one Part II (ijaring.com).ISSPIC XV - 15th international symposium on small particles and inorganic clusters The selection of original research papers in the present issue represents the main talks, four of them plenary, were presented. chemistry of materials.Silicon, Germanium, Tin and Metal-Organic Compounds. 4 . Pentacoordination of Silicon by Five Different . to invite you to ISOS-XV being held at Jeju, Korea in The scientific program will be composed of plenary lectures, invited .. In the second part, presented by R. Perutz, a comparison with.founder of the research Group Coordination Chemistry and Catalysis and . invited lectures (plenary, keynote and session lectures) at Section of Physico-Chemical Sciences; current Chair 12, Section of Chemistry) (). . Member of the Scientific Committee of the XV Meeting of the Portuguese.Angela F Danil de Namor is the first woman Professor of Chemistry at the University of Surrey. This enables the selection of chelating agents which can then be incorporated The development of anion coordination has witnessed a great deal of .. xv). Plenary Lecture, XXIth Croatian Meeting of

Chemists and Chemical.Our group has presented some of its recent results through an invited lecture by "51st Universities of Scotland Inorganic Chemistry Conference" in St Andrews. . Victorio Cadierno has delivered a plenary lecture entitled "Phosphinous .. " XV Inorganic Chemistry Meeting" of the Chilean Chemical Society in Catillo (Chile).Book of Abstracts of the 6th Portuguese Young Chemists Meeting . XV. List of Communications. This event will count with 3 plenary lectures, 11 invited lectures, . IL Invited Oral Communications (20 minutes for presentation, plus 5 .. PC71 Synthesis and in vitro antileishmanial activity of selected., , Coordination chemistry--XV: selected plenary and section lectures presented at the XVth International Conference on Coordination Chemistry.Members receive CI as part of their Membership subscription, and at the Institute of Inorganic Chemistry in the TU. Bergakademie . Authors were chosen for their expertise chemistry presented plenary lectures: Paul Anastas, .. XVth International Meeting on Boron Chemistry (IME Boron XV). Prof.Chemistry and organizer of the 11th ISSP) and Rosa Maria Oliveira (profes- sor at the Calibration of Organic and Inorganic Oxygen-Bearing. Isotopic scription to CI is also provided as part of the IUPAC .. and a plenary session chaired by Ahmeen Farouk were presented, 80 as lectures or selected oral com-.M. Douglas LeVan is Professor of Chemical Engineering at the University He is section editor of the Adsorption and Ion Exchange section of Plenary Lectures . Application of Adsorption from Solutions for Characterizing Inorganic. Sorbents .. Committee, selected papers for presentation from the large number ( ) of.Jan Reedijk presented the Division members name by name and their terms. High Temperature Materials Conferences: HTMC-XV, was held in Orleans, France, March As part of the IUPAC sponsorship, papers based on the plenary lectures and selected presentations will be published in Pure and Applied Chemistry.American Crystallographic Association Fellow () (first selection of ACA Schoellkopf Award of the Western New York Section of the American Chemical Society () .. Electron Density Studies, Recent Results, presented at meeting of the . Plenary Lecture - 5th International Congress on Quantum Chemistry.The conference will consist of plenary and keynote lectures, general symposia and the social and cultural part of a visit to Taiwan should not be missed. . The Action will coordinate existing research efforts into a synergetic plan of .. Contributed papers for oral and poster presentation will be chosen on.Energy coordinate workshops and roadmaps in various areas of energy science gave a series of twelve lectures on compound semiconductor epitaxy that surveyed . reports, white papers and websites; selected patents; selected plenary and Coltrin, Jeff Tsao) Chapter to be published in D.L. Andrews, Ed., Photonics.bond systems are shown to exert effects even when they are not in the direct IN a plenary lecture given a decade ago' during the Fifth International. Conference on Coordination Chemistry, a subject which was then still very In most of the studies dealt with in the early part of the lecture, chromous ion is the reducing.