RELATIVISTIC EFFECTS IN ATOMS, MOLECULES, AND SOLIDS pdf

1: Relativistic many-electron Hamiltonians - IOPscience

The NATO Advanced Study Institute (ASI) on "Relativistic Effects in Atoms, Molecules and Solids" cosponsored by Simon Fraser University (SFU) and Natural Sciences and Engineering Research Council of Canada (NSERC) was held at the University of British Columbia (UBC), VanÂ- couver, Canada from.

Is that the case for all atoms? And what about molecules and crystals? Before we answer these questions rigorously, let us try to answer them intuitively. Consider for example the hydrogen molecule, H2. It is made of two hydrogen atoms sharing their electrons. Since the size of the two hydrogen atoms taken separately varies with the Bohr radius, it would be reasonable to expect the size of the hydrogen molecule to do the same. If the radius of all atoms depended on the Bohr radius, we could apply the same reasoning to all molecules and crystals. Intuitively, we would arrive to the conclusion that the dimensions of matter depend on the Bohr radius. If this were to be the case, then according to chapter one, the size of any object would be different depending on its location in a gravitational potential. In this appendix, we will see how the dimensions of matter are predicted to vary theoretically. We will first look at all atoms. We will then study molecules which will be followed by crystals and metals. Until now, ao has always been considered a constant because ,eo, e and me have been supposed constants. For an experimentalist, by definition, that numerical value is equal to one bohr unit whether the electron orbit in hydrogen is constant or not. For theoretical results, this is different. Theoreticians could decide to give the results of their calculations in function of ao i. For the theoreticians, ao is defined as a combination of parameters. Therefore ao is constant only if all the parameters are constant. One then has to be careful in reading theoretical results and look at the method used to see if there really is a dependence of ao or if it is just a unit. Let us make sure that the physics is not lost in those calculations. Most authors do their calculations in atomic units. This means that the unit of mass is the electron mass. The authors then go on with numerical calculations to solve the equations. But if the mass of the electron is not a constant, then it is not necessarily equal to one in atomic units with respect to the initial frame of reference. All the results in this appendix being theoretical, we made sure that their dependence in ao was real. ATOMS - It is easy to derive the radius of all hydrogenlike atoms by supposing that they are just like a hydrogen atom with an electron orbiting a nucleus of charge Z. According to Levine [1] page The radius of all other atoms has been well investigated [2, 3] and the results given are proportional to the Bohr radius. The method used in [2] was the Hartree-Fock method [4] and in [3] , the Dirac-Fock method which is just the Hartree-Fock method with relativistic corrections due to the mass of the electron with respect to the nucleus frame of reference. The Dirac-Fock method gives no relativistic correction of the electron mass with respect to an external gravitational potential. Upon finding its wave function and the potential of the nucleus in the Born-Oppenheimer approximation , it is possible to calculate the distance between the two protons. The variational method is used to solve this problem [5]. It uses wave functions of the hydrogen atom which depend on the Bohr radius. The internuclear distance of a molecule is in direct relationship with the size of that molecule. We see then that the size of the hydrogen molecule ion is proportional to ao. This means that when we change the mass of the particle moving about the nucleus, the size of the hydrogen molecule ion also changes. This has already been realized by Levine [1] page When a beam of negative muons produced when ions accelerated to high speed collide with ordinary matter enters H2 gas, a series of processes leads to the formation of muomolecular ions that consist of two protons and one muon. Its Re [the distance between the two protons] is 2. If one day we are able to produce a molecule with a proton and an anti-proton, the internucleus distance of that molecule will be amazingly small. It is obvious from this result that the size of the hydrogen molecule ion depends on the electron mass. For heavier molecules, the calculations were done using internal relativistic corrections [10, 11, 12] because of the higher mass of the electron. Relativistic corrections due to an external gravitational potential were never taken into account. All the results cited in the references are in units of ao or in units that are related to ao and are proportional to ao. The constant of proportionality depends only on the structure of the crystal. This means that the size of crystals is proportional to the Bohr radius since we have seen in the previous section that the size of all molecules and thus the distance between

the nuclei in diatomic molecules is proportional to the Bohr radius. Furthermore, the same author [13] pages develops an ionic model for metals. According to this model, the atomic radius in a metallic crystal which is defined as half the shortest interatomic distance can be expressed as: We see then that the size of metals is proportional to the Bohr radius as defined in chapter one. This means that, since every object we know is made of either atoms, molecules, crystals or metals, the results of chapter one concerning the dilation and contraction of the Bohr radius in the hydrogen atom apply to all matter including humans. Finally, we conclude that this dilation or contraction is real. Lee and Kenneth S. Jeffrey Hay, Richard L. Martin et Frank W. Wadt et Luis R. Malli editor, Plenum Press, New York, page , Ross et Phillip A.

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2: Relativistic and Electron Correlation Effects in Molecules and Solids : G. L. Malli :

This book contains the main lectures (as well as abstracts of additional lectures) given at the NATO Advanced Study Institute (ASI) on "Relativistic Effects in Atoms, Molecules and Solids," whose purpose was to discuss and review recent developments in the relativistic many-electron problems in.

The calculations further demonstrate that relativistic and electron correlation effects are nonaddi- tive. The measured dipole polarizabilities of Sn and Pb are in reasonable agreement with the theoretical values. Recent advances on the experimental side include time- value from 80 a. This is due to a large direct led to a considerable improvement in the accuracy for the relativistic 6s-shell contraction. But classical molecular istic effects are much less pronounced, i. As the spin-orbit theoretical side one faces the difficulty of correctly describ- splitting becomes very large for the heaviest p-block ele- ing electron correlation and relativistic effects, as the latter ments in the periodic table, we expect that such effects will increase substantially with increasing nuclear charge Z considerably influence the dipole polarizabilities. While closed-shell atoms and ions have been studied fill the gap for open-shell polarizabilities, we decided to un- extensively in the past, and accurate polarizabilities are dertake accurate nonrelativistic and relativistic coupled clus- available for most of these elements, open-shell species are ter calculations for all group atoms in their 3 P0 ground far more difficult to treat as often a multireference procedure state. If analytical procedures were not available for the calculation of the polarizability tensor, we used a finite field method instead. In this case fields of 0. For the open-shell procedure we used spin unrestricted Hartree-Fock and Kohn- Sham theory. We applied extensive, uncontracted Gaussian- type basis sets, which were thoroughly tested to yield con- verged polarizabilities with respect to basis set extension towards softer and harder functions at the coupled cluster level. For these elements we used the full active orbital space in our electron correlation procedure. Here we beam profiles are fitted with Gaussian functions. Finally, we considered the Gaunt term. Perdew and Cole implemented the III. We there- mentally determined utilizing a molecular beam electric field fore decided to evaluate the Gaunt interaction to the polariz- deflection apparatus, previously described in the literature ability at the Dirac-Hartree-Fock level of theory only. In our experiments on and co-workers are 2. Further, very recent results at the tightly collimated and passed through an inhomogeneous Dirac-Coulomb level of theory for the heaviest elements Pb electric field, where it gets deflected. This gives us confidence for the accuracy of all beam profile and detecting transmitted atoms with a time-of- our results. For this purpose the atoms are ion- Figure 2 compares the calculated polarizabilities at the HF ized with a F2-excimer laser. We make the following observations: The mean velocity of tin, lead, and not even negligible for carbon. This leads to the higher contribution increases with nuclear charge and, for the three velocities of the tin atoms and thereby reduced deflections in heaviest elements, cannot be neglected anymore in precise the electric field. For example, we see a The most accurate coupled cluster results including the change from The recommended polariz- p-block elements. There are some notable failures in the past. More recent calculations with As their values are slightly smaller compared to ours, we list larger basis sets and a variety of different functionals give a theirs, however, correcting them with our calculated Gaunt better comparison, i. In our case, all functionals over- relativistic but also the spin-orbit correction has to be taken estimate the dipole polarizability by a few atomic units. In- into account, in order to reproduce the experimental data. We note that the overestimation is propor- tings and low temperatures. All values are in a. We thank Daniel procedure. Benker for helpful discussions. Atoms, Molecules and Clusters, edited mond, and D. Fundamentals, edited by P. Schwer- edited by D. Sin Fai Lam, J. A , Toyota, R.

3: Atoms and molecules in relativistic quantum mechanics - IOPscience

Proceedings of a NATO Advanced Study Institute on Relativistic Effects in Atoms, Molecules, and Solids, held August 1 , 1 , at the University of British Columbia, Vancouver, Canada.

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4: The Dependence of the Size of Matter on Electron Mass

Preface Recent years have seen a growing interest in the effects of relativity in atoms, molecules and solids. On the one hand, this can be seen as result of the growing awareness of the.

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