

MOLECULAR ELECTRONIC STRUCTURES WITH THE MOLPRO PACKAGE

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INTRODUCTION

Theoretical simulations involve using mathematical and computational models to simulate and predict the behavior and properties of a system. Theoretical simulations allow scientists to explore the behavior of a system under different conditions, and can provide insights into the fundamental principles that govern the system's behavior, while experimental methods, on the other hand, involve directly measuring the physical properties of a system using various laboratory techniques. Studying various computational simulations allows us determine physical and chemical properties and quantities of atoms or molecules. Molpro[1-2] is one of the a useful software package for electronic structure calculations including electronic structures, potential energy surfaces, spectroscopic properties, and reaction mechanisms of molecules and materials.

Sodium hydride (NaH) is chosen to investigate the electronic structure properties. NaH is a simple ionic compound consisting of a sodium cation (Na⁺) and a hydride anion (H⁻). In terms of its electronic structure, NaH is a polar covalent compound with a predominantly ionic character. The sodium cation donates an electron to the hydride anion, forming an ionic bond. However, there is also a significant degree of covalent character, as the hydride anion contains a partially negatively charged hydrogen atom that can form weak covalent bonds with other atoms or molecules. Calculating potential energy surfaces (PESs), dipole moments (DMs), and transition dipole moments (TDMs) are important because they provide fundamental information about the electronic and nuclear properties of molecules and materials, which are crucial for understanding their behavior and properties.

RESULTS AND DISSCUSTION

The potentials employed for our calculations are depicted in Fig. 1. During the calculating we have chosen the as augmented quadruple zeta (AVQZ) basis set, the method is the Multi-configurational Self-Consistent Field (MCSCF). In all calculations the internuclear distance between Na and H atoms are 1.8 to 18 atomic unit (a.u.). It is evident from Fig. 1 that the B state is a repulsive potential while the X and A potentials support bound vibrational states. The total energie (PES) for individual electronic states can be written in term of semiclassical approach [4-5]:

$$\hat{E} = \hat{T}_e + \hat{T}_n + \hat{V}_{ee} + \hat{V}_{en} + \hat{V}_{nn} \quad (1)$$



where T_e and T_n are kinetic energies of each electron and nucleus, V_{ee} , V_{en} and V_{nn} are the potential energies between electron-electron repulsion, electron-nuclear attraction and nuclear-nuclear interaction, respectively. The values of PESs obtained by using the Molpro software [2] are almost the same as shown in [3] reference, which means that our obtained results are reasonable. We have used the GNUPLOT package to plot our figures.

In addition, the variation of permanent dipole moments (DM) are obtained and shown in Fig. 2 by the help of Molpro software. The permanent dipole moment of a molecule in terms of quantum mechanics is given by the expectation value of the electric dipole operator, which is defined as:

$$\mu = \langle \Psi | \hat{\mu} | \Psi \rangle \quad (2)$$

where $\hat{\mu}$ is the electric dipole operator, Ψ is the wave function of the electronic state of the molecule. For example, while calculating DM for ground state, $\hat{\mu}$ and Ψ are ground state electric dipole operator and ground state wave function. XX, AA and BB in the Fig. 2 stand for dipole moments between ground states, first and second excited states, respectively. It is clear that dipole moment of second excited state (B) is almost negligible, while dipole moment of Ground (X) and first excited (A) states are relatively large. The dipole moment of a molecule's curtain electronic

state can provide important information about the distribution of charges within the molecule, which can in turn influence the molecule's chemical and physical properties: if the dipole moment of a particular electronic state is large, it suggests that there is a significant separation of charge within the molecule, which may be due to the presence of polar bonds or a highly asymmetric molecular structure, on the other hand, if the dipole moment of a particular electronic state is very small, it suggests that the molecule has a more uniform distribution of charge, which may

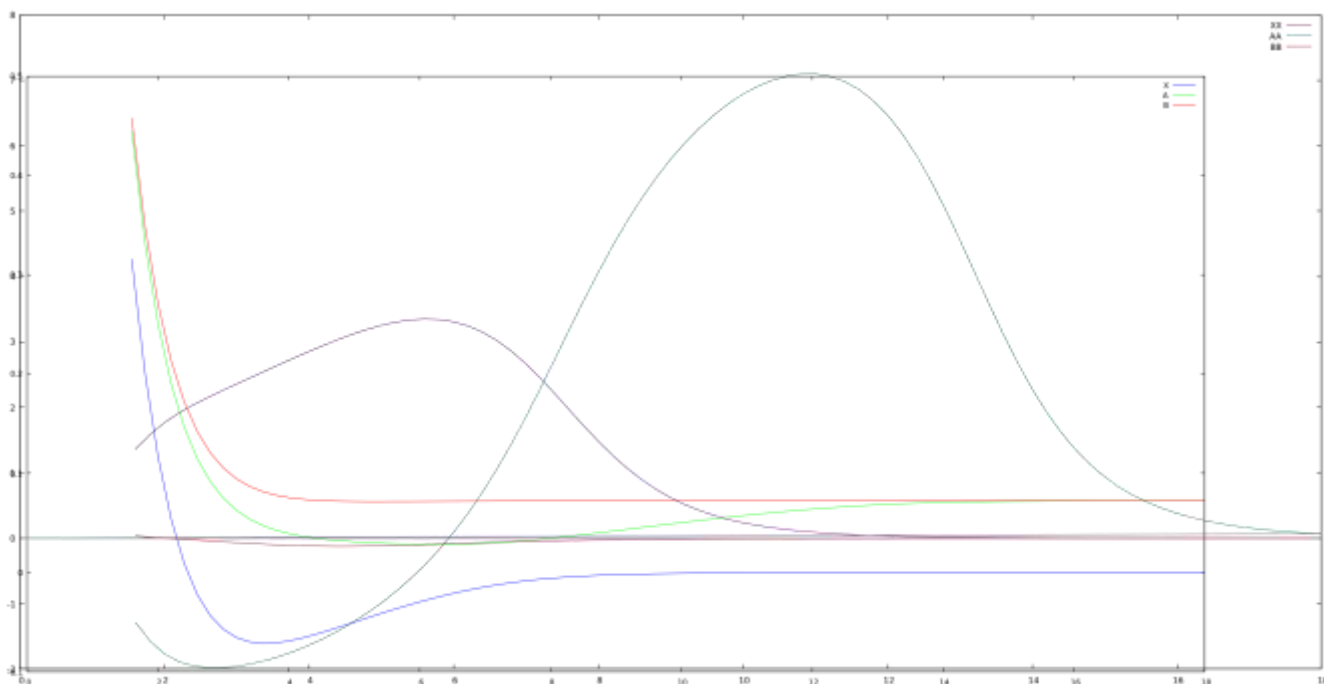
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small, it suggests that the molecule has a more uniform distribution of charge, which may be due to the absence of polar bonds or a symmetric molecular structure.

Fig. 1. Potential energy surfaces of three singlet electronic states of NaH molecule. Blue curve (X) is a ground state, while green (A) and red (B) ones correspond to first and second excited states of the NaH system.

The third plot describes as the same figure as first one, but except for one extra curve so-called shifted ground state of the system. It can be really useful to calculate the simulations of



molecular dynamics with MCTDH [6-7] or other packages. In the subsequent works we may study molecular dynamics like kinetic release energies, populations and autocorrelation of these states of NaH with the MCTDH package.

Fig. 2. Permanent dipole moment of three singlet electronic states of NaH molecule. XX, AA and BB stand for dipole moments between ground states, first and second excited states, respectively.

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