Accurate *ab initio* calculations of interaction potentials of the alkali and alkaline-earth hydrides

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Simple diatomic molecules play an important role in quantum chemistry and physics by providing the playground for benchmarking molecular theory and implementing quantum control. Precise calculations of molecular properties are crucial for guiding ongoing experiments and for planning new ones. Ultracold molecules provide a good framework for observations of quantum effects and testing various theories. Alkaline-earth-metal monohydrides are also promising candidates for a source of ultracold hydrogen [1] and laser cooling to ultralow temperatures [2].

Calculations of potential energy curves are a groundwork for determining other molecule properties such as rovibrational states. Neutral alkali and alkaline-earth monohydrides have already been extensively studied by others [3], unlike their ions. Experimental spectroscopic studies on the BaH^{2+} molecule are currently underway in Prof. F. Merkt's group at ETH Zurich, where recently BaH^+ and BaD^+ were studied [4]. Here, we aim to provide the interaction energies for all neutral and ionic alkali and alkaline-earth hydrides as accurately as possible using various methods and basis sets.

We applied coupled cluster theory (CCSD, CCSD(T), CCSDT and MRCCSD) for post-Hartree-Fock calculations. A range of different electronic structure techniques was employed to achieve a high level of accuracy and provide insightful comparisons. Basis sets with cardinal numbers up to 5Z were utilized and the energies were extrapolated to the complete basis set limit. We applied corrections such as the diagonal Born-Oppenheimer correction (DBOC) and the correction for the full triple excitations in the coupled cluster calculations. Potential energy curves were calculated for distances ranging from 2 a_0 up to 50 a_0. Adopted corrections helped us improve the accuracy of our results. Additionally, the DBOC correction was also calculated for other alkaline earth metal monohydride ions. We reached a theoretical accuracy of around 0.5% - 1.5% at the minimum.

The results of our calculations are highly accurate and serve as a strong foundation for deriving other molecular parameters. The ionized alkaline-earth hydrides have not been extensively studied by others in terms of *ab initio* calculations and our results are among the most accurate available. Additionally, they provide a valuable reference for comparison with experimental data.

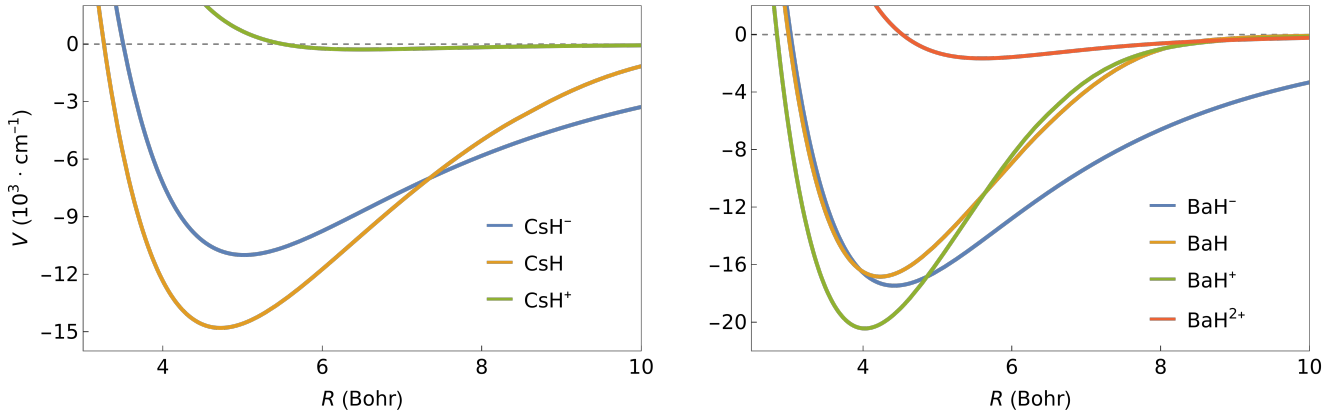

Figure 1: PECs of ionic and neutral hydrides of Cs and Ba.

References

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