

## عنوان مقاله:

+Ab initio potential energy curves and transition dipole moments for the low-lying electronic states of GeH

## محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 2

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## خلاصه مقاله:

The germanium hydrides containing GeH<sub>n</sub> and GeH<sub>n</sub><sup>+</sup> are important source materials for the growth of semiconductor films using chemical vapor deposition method. The GeH<sup>+</sup> cation have been the topic of many theoretical and experimental investigations that focused on its spectroscopic properties. The a<sup>3</sup>Π-X<sup>1</sup>Σ<sup>+</sup> and A<sup>1</sup>Π-X<sup>1</sup>Σ<sup>+</sup> band systems of GeH<sup>+</sup> have been recorded in emission [1-3]. Since GeH<sup>+</sup> contains the heavy atom Ge, the effect of spin-orbit coupling (SOC), which may play a significant role in the spectroscopic and dynamic characterizes of electronic states, should be considered. In a very recent theoretical study [4], multi-reference configuration interaction was used for 8 Λ-S states and 23 Ω states of GeH<sup>+</sup>: Ge+(2P<sub>o</sub>) + H(2S) → 1,3Σ<sup>+</sup>, 1,3Π that made the ground state asymptote and Ge+(4P) + H(2S) → 3,5Σ<sup>-</sup>, 3,5Π, which lies at 51600 cm<sup>-1</sup> above the ground state asymptote. However, the two asymptote Ge(3P)+H+(1S) → 3Σ<sup>-</sup>, 3Π and Ge(1D) + H+(1S) → 1Σ<sup>+</sup>, 1Π, 1Δ lie at about 46000 and 53090 cm<sup>-1</sup> above the ground state asymptote, respectively; the electronic states of these second asymptote were ignored in Ref. [4]. In this work we considered 13 Λ-S states and 50 Ω states of GeH<sup>+</sup> and plotted potential energy curves, dipole moments and transition dipole moments between different electronic states with spin-orbit coupling.

## کلمات کلیدی:

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