Développement d'un potentiel modèle ab initio par la méthode de perturbation Van Vleck pour l'étude spectroscopique de molécule Ak-Rg

Doctorant·e
HOCHARD Erwan

Direction de thèse
GERVAIS BENOIT (Directeur·trice de thèse)
DOUADY Julie (Co-encadrant·e de thèse)

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Rapporteurs de la thèse
DULIEU OLIVIER Université Paris Saclay
JEANMAIRET GUILLAUME Sorbonne Université

Membres du jurys
DOUADY Julie, , UCN - Université de Caen Normandie
DULIEU OLIVIER, , Université Paris Saclay
GERVAIS BENOIT, , UCN - Université de Caen Normandie
JEANMAIRET GUILLAUME, , Sorbonne Université
LABEYE MARIE, , ENS-PSL
VIEL ALEXANDRA, , UNIVERSITE RENNES 1

Abstract

In this thesis, we develop an ab initio potential model based on Van Vleck perturbation theory for the spectroscopic study of alkali–rare gas (Ak-Rg) molecules. By combining perturbation theory with advanced modeling methods, we construct accurate interaction potentials to analyze the electronic structure and spectroscopic properties of the studied molecular complexes. Special attention is given to core-valence correlation and relativistic effects, which are crucial for a rigorous description of interatomic interactions involving heavy atoms. We explore the applicability of the model in the context of excited-state spectroscopy, emphasizing the vibrational levels and electronic transitions of Ak-Rg molecules. The obtained results are compared with experimental data and existing ab initio calculations, highlighting the relevance and accuracy of the developed method. This approach opens new perspectives for modeling complex interactions in molecular systems involving alkali and rare gas elements.