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An *ab initio* investigation on the low-lying electronic states of NaMg

Song Li[a,*], Ming-Jie Wan[b], Shan-Jun Chen[a], Yuan-Yuan Jin[a],

Chuan-Zhao Zhang[a], Peng Chen[a], Ning Wang[a]

[a] *School of Physics and Optoelectronic Engineering, Yangtze University, Jingzhou, China*

[b] *Computational Physics Key Laboratory of Sichuan Province, Yibin University, Yibin, China*

* Corresponding author: Song Li
School of Physics and Optoelectronic Engineering
Yangtze University
Nanhuan Road 1, Jingzhou
China
E-mail: lsong@yangtzeu.edu.cn
Tel: +86 716 8060942

Abstract: Theoretical investigations for NaMg have been performed on the icMRCI+Q level employing basis set of quintuple-ζ quality with corrections of core-valence correlation and scalar relativistic effect. The geometrical parameters, potential energy curves, vibrational energy levels, spectroscopic constants for the eight Λ-S states, with respect to the lowest four dissociation limits, are investigated. Through the spin-orbit coupling effect, these states split into fourteen Ω states. The permanent dipole moments, transition dipole moments, Einstein emission coefficients, radiative lifetimes and Franck-Condon factors for all Ω states are studied. The feasibility of performing laser cooling of NaMg has also been discussed. Our predictive results are anticipated to serve as guidelines for further researches on NaMg.

Keywords: NaMg; *ab initio* calculations; electronic structure; spin-orbit couplings; spectroscopic constants