1 - 5 *Ab initio* Calculations for Isospin Symmetry Breaking in Nuclear Systems*

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In the present work, we utilize the approach of the *ab initio* valence-space in-medium similarity renormalization group (VS-IMSRG) to investigate isospin-symmetry breaking in medium mass nuclei. The adopted nuclear force incorporates charge-symmetry and charge-independence breakings. We focus on computing mirror energies of *sd*- and *pf*-shell nuclei and discuss the influence of single-particle states, particularly those with s-wave character, on weakly bound and unbound nuclear states of *sd*-shell nuclei. To demonstrate the predictive capability of our *ab initio* VS-IMSRG calculations, we also perform mean excitation energies (MEDs) calculations in a large set of *sd*-shell nuclei(Fig. 1). The left panel of the figure presents pairs of states with the highest experimental MED values. These results show that the VS-IMSRG method provides a reliable description of the properties of *sd*-shell nuclei. Additionally, we present results obtained using *ab initio* VS-IMSRG based on the NN + 3N interaction. The calculated spectra exhibit excellent agreement with experimental energies. Both the experimental and theoretical values reveal that the MED and total excitation energy differences (TED) are on the order of several tens and hundreds of keV, respectively. The MED values demonstrate satisfactory agreement between *ab initio* VS-IMSRG calculations and experimental data, although there is a slight discrepancy for $J = 2, 4$ many-body states. In contrast, our calculations consistently yield TED values approximately 100 keV larger than the corresponding experimental data.

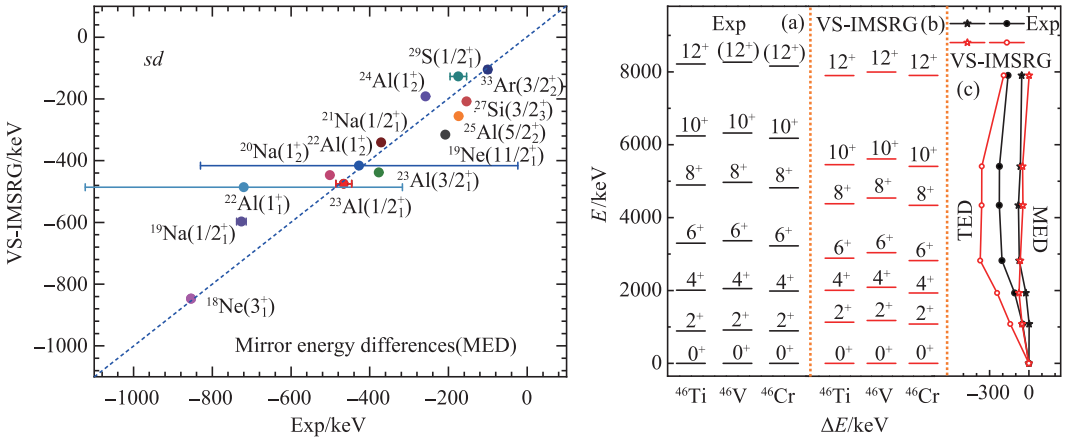

Fig. 1 (color online) The left panel is the calculated MEDs with *ab initio* VS-IMSRG, labeled with the name of the associated proton-rich nucleus, are compared with experimental data. The right panel is Yrast states with $T = 1$ in ^{46}Ti, ^{46}V and ^{46}Cr. (a) provides their excitation energies from experimental data, (b) shows the calculated excitation energies using *ab initio* VS-IMSRG with the 1.8/2.0 (EM) NN + 3N interaction, (c) shows MED and TED (mirror and triplet energy difference) values as a function of the angular momentum J (the shown angular momenta correspond to the calculated angular momenta in the spectrum of ^{46}Cr). The black full stars (red open stars) denote the experimental (*ab initio* VS-IMSRG) MED values, while black full dots (red open dots) refer to the experimental (*ab initio* VS-IMSRG) TED values.

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