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DATA PAPER

Mutual neutralization in low-energy collisions of $Na^+ + H^-$ ions

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The low-energy mutual neutralization (MN) reactions $Na^+ + H^- \rightarrow Na(nl) + H$ have been studied by employing the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method over a wide energy range of 10^{-3}–10^3 eV/u. Total and state-selective cross sections have been investigated and compared with the available theoretical and experimental data, and the state-selective rate coefficients for the temperature range of 100–10000 K have been obtained. In the present work, all the necessary highly excited states are included, and the influences of rotational couplings and 10 active electrons are considered. It is found that in the energy below 10 eV/u, the Na(4s) state is the most dominant exit state with a contribution of approximately 78% to the branch fraction, which is in best agreement with the experimental data. For energies above 10 eV/u, the MN total cross section is larger than those obtained in other theoretical calculations and shows a slow decreasing trend because the main exit states change, when the energy is above 100 eV/u, the dominant exit state becomes the Na(3p) state, while the Na(4s) state becomes the third most important exit state. The datasets presented in this paper, including the potential energy curve, the radial and rotational couplings, the total and state-selective cross sections, are openly available at https://doi.org/10.57760/sciencedb.j00113.00112.

Keywords: mutual neutralization, cross section, rate coefficient, quantum-mechanical molecular-orbital close-coupling (QMOCC) method

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1. Introduction

The low-energy mutual neutralization (MN) reaction between alkali metal positive and hydrogen negative atomic ions has significant importance in controlled fusion plasmas, astrophysics, and other related fields. For example, the MN process is important in diagnostics of fusion plasmas and experiments involving negative ions,[1,2] particularly the reactions involving H^- ions are of great interest in ion sources in tokamaks.[3] On the other hand, in modern astrophysics, to accurately determine the abundance of elements in a star, the MN process between alkali metal positive atomic ions with hydrogen anions must be taken into account with the non-local thermodynamic equilibrium (non-LTE) effects.[4,5]

Sodium and hydrogen are essential elements in both plasma and astrophysics, and the significance of the low-energy MN reaction ($Na^+ + H^- \rightarrow Na(nl) + H$) between Na^+ and H^- ions has long been recognized in the atomic physics community. In recent years, Barklem *et al.* emphasized the importance of these processes in stellar atmospheres.[6] Despite the universal importance of such MN reactions, there have been very few experimental studies on these processes, and only recently Eklund *et al.* reported the merged-beam experiments about mutual neutralization reactions between Na^+ and D^- ions using the DESIREE ion beam storage ring, providing branching ratios for the main reaction states of Na(4s, 3d, and 4p) over energies ranging from 80 meV ($\sim$ 43 meV/u) to 393 meV ($\sim$ 214 meV/u).[7]

Many astrophysical and laboratory plasmas (including the edge plasma of thermonuclear fusion devices), in which the typical collision energy range from 0.01 eV/u to several hundred eV/u (or to the keV/u region for some heavy-particle collision processes),[8] still face challenges in the theoretical study of MN processes between Na^+ and H^-. In particular, the most reliable full quantum methods dealing with the low-energy collisions are currently facing challenges due to the high energy levels of the initial ionic state, and the strong couplings between different states. The only fully quantum (FQ) method is from Dickinson *et al.*,[9] who determined a quantitative description of relative motion and provided total and state-selective cross sections for collision energies of 0.01–100 eV/u, However, only two active electrons were considered and the influence of rotational couplings was not contained in their work.

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For the collision energy below 10 eV/u, most researchers have studied the MN collision mechanism based on the Landau–Zener (LZ) dynamics of the avoided ionic curve crossing mechanism but with different methods to calculate the coupling at the avoided crossings. For example, Olson *et al.* used semiempirical (SE) couplings,[10] Janev *et al.* determined the couplings by using the Landau–Herring method,[11] and Barklem employed a two-electron linear combination of atomic orbitals (LCAO) method.[12] As the collision energy increases and the interacting nuclear distance R decreases, more couplings between states need to be considered in the small R region, the LZ method only considers the most important avoided crossings. At higher energy region, Olson *et al.* employed pseudopotentials and solved the perturbed stationary-states coupled-channel equations to get the cross sections for the 0.1–5.0 keV/u energy region.[13] In the work of Errea *et al.*, a five-state molecular expansion with the inclusion of two-electron translation factors has been used to calculate the neutralization cross sections for 0.16–5 keV/u.[14] However, in their works, the influence of higher excited states (e.g., Na(3d/4p)) was ignored, and these states were later found to be non-negligible in the subsequent studies.[7] In a word, in the energy range of 10^{-3}–10^{3} eV/u required for the plasma and astrophysics modeling, there still exist obvious differences between theoretical and experimental results.

In this paper, the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method is used to study the neutralization process $Na^{+}+H^{-}\rightarrow Na(nl)+H$ over a quite wide energy range from 10^{-3} eV/u to 10^{3} eV/u. The calculated cross sections are compared with experimental data, and possible reasons for discrepancies with previous calculations are discussed. The electronic structure parameters are necessary for the dynamical calculations,[15,16] including adiabatic potentials, radial and rotational coupling matrix elements. In this paper, they are calculated using the *ab initio* multi-reference single- and double-excitation configuration interaction (MRD-CI) method.[17,18]

The organization of this paper is as follows. In Section 2, the *ab initio* calculation of molecular potential energy surfaces and coupling data are presented. In Section 3, we analyze the scattering calculation results and discuss the differences with the available experimental and theoretical results. Finally, we provide a brief summary in the last section. Unless otherwise stated, atomic units are used throughout this paper.

2. Electronic structure calculation

In the present work, the multi-reference single- and double-excitation configuration interaction (MRD-CI) method[17,18] is used to calculate the potential energy curves and coupling data of seven $^{1}\Sigma^{+}$ and three $^{1}\Pi$ electronic states for the quasi-molecular system (NaH) in A_1 and B_1 symmetries (C_{2v}), respectively. The $^{1}\Delta$ states have been disregarded since the initial state ($Na^{+}+H^{-}$) is a $^{1}\Sigma^{+}$ state and such effects are quite small. An effective core potential (ECP) adapted basis set (4s, 4p, 2d, 1f)[19] is used for the Na atom, with a relatively large diffuse basis set (5s4p2d1f) employed to describe its Rydberg states. While the hydrogen atom is described using a correlation-consistent polarized valence quadruple-zeta (cc-pVQZ) Gaussian (6s, 3p, 2d, 1f) contracted to [4s, 3p, 2d, 1f],[20] along with a diffuse (1s1p) basis set. These MRD-CI calculations are performed with a threshold of 5.0×10^{-8} Hartree (1.36×10^{-6} eV) and a range of nuclear separations from 2.00 a.u. to 100.00 a.u. The calculated energies in the asymptotic region are shown in Table 1 and compared to experimental data from the National Institute of Standards and Technology (NIST)[21] with an error of less than 0.050 eV, and this accuracy should be sufficient for the scattering calculations.[22] The highly relevant electronic wave functions are then employed to compute the radial and rotational coupling matrix elements by using finite differentiation and analytical approaches, respectively.[23]

Table 1. Asymptotic separated-atom energies for the states of NaH system. The bold 7 $^{1}\Sigma^{+}$ represents the initial state.

Molecular states	Asymptotic atomic states	Energy (eV)		
		MRD-CI	Exp.[21]	Error
$1\,^{1}\Sigma^{+}$	$Na(2p^{6}3s\,^{2}S)+H(1s^{2}S)$	0.000	0.000	0.000
$2\,^{1}\Sigma^{+}$, $1\,^{1}\Pi$	$Na(2p^{6}3p\,^{2}P^{o})+H(1s^{2}S)$	2.067	2.102	0.035
$3\,^{1}\Sigma^{+}$	$Na(2p^{6}4s\,^{2}S)+H(1s^{2}S)$	3.148	3.191	0.043
$4\,^{1}\Sigma^{+}$, $2\,^{1}\Pi$	$Na(2p^{6}3d\,^{2}D)+H(1s^{2}S)$	3.616	3.617	0.001
$5\,^{1}\Sigma^{+}$, $3\,^{1}\Pi$	$Na(2p^{6}4p\,^{2}P^{o})+H(1s^{2}S)$	3.716	3.752	0.036
$6\,^{1}\Sigma^{+}$	$Na(2p^{6}5s\,^{2}S)+H(1s^{2}S)$	4.066	4.116	0.050
$7^{1}\ \Sigma^{+}$	**$Na^{+}(2p^{6}\,^{1}S)+H^{-}(1s^{2}\,^{1}S)$**	**4.374**	**4.385**	**0.011**

The adiabatic potentials of NaH quasi-molecule as a function of internuclear distance $R=2.00$–50.00 a.u. are shown in Fig. 1 corresponding to Table 1. The 7 $^{1}\Sigma^{+}$ state represents the initial ion state $Na^{+}(2p^{6}\ ^{1}S)+H^{-}(1s^{2}\ ^{1}S)$. In this work, we do not consider higher excited states, e.g., Na(4d/4f/5p) + H, these higher lying states create covalent molecular NaH states, which either produce non-adiabatic regions at large internuclear distances (i.e., the pseudo-crossing between ionic and neutral states at $R>100.00$ a.u.) or do not produce avoided crossings at all. While the interaction range

for low-energy collisions of alkali metal and H^- ions is within $R < 100.00$ a.u., and the scattering cross sections of these states are quite small.[24] It can be seen that there are strong pseudo-crossings between the 4 and 5 $^1\Sigma^+$ states and between the 5 and 7 $^1\Sigma^+$ states at $R \sim 34.20$ a.u. and 38.50 a.u., respectively, and a strong and broad avoided crossing exists between the 3 and 4 $^1\Sigma^+$ states near $R \sim 22.00$ a.u., these may have a significant effect on low-energy mutual neutralization processes. It should be notable that as $R < 5.00$ a.u., with the internuclear distance R decreasing, the potential curves of the ionic and neutral states become increasingly close, which implies that the broad radial and rotational couplings may be important for mutual neutralization processes in higher collision energy region.

In this work, the radial and rotational coupling matrix elements between all pairs of states have been calculated, and they are transformed into[25]

$$\begin{aligned} &\langle \psi_K | \partial/\partial R - (\varepsilon_K - \varepsilon_L) z^2/2R | \psi_L \rangle, \\ &\langle \psi_K | \mathrm{i}L_y + (\varepsilon_K - \varepsilon_L) zx | \psi_L \rangle, \end{aligned} \tag{1}$$

respectively. In these equations, ε_K and ε_L represent the electronic energies of states ψ_K and ψ_L, and z^2 and zx represent the components of quadrupole moment tensor. The correction form used here is similar to the correction obtained using the electron translation factor (ETF) method.[26]

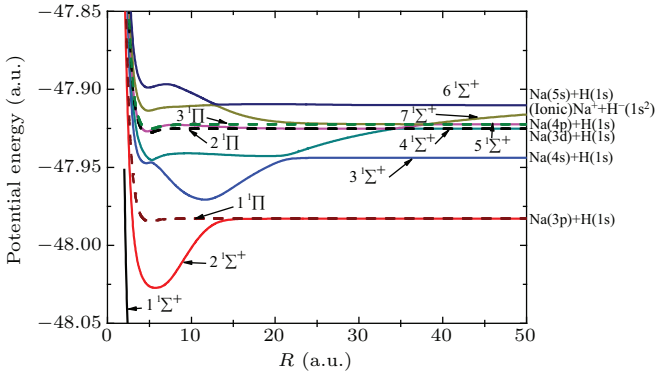


Fig. 1. Potential curves of NaH molecule refer to Table 1. The solid and dashed lines represent the $^1\Sigma^+$and $^1\Pi$ states, respectively.

Figure 2(a) shows some important radial coupling matrix elements, whose peak positions coincide with the avoided crossing in Fig. 1. Around $R \sim 22.00$ a.u., there exists a strong and broad coupling between the 3 and 4 $^1\Sigma^+$ states, this coupling should be the primary gateway of electron charge-transfer flux toward the exit states. At $R < 15.00$ a.u., some obvious strong couplings can be observed, such as the couplings between the 2 and 3 $^1\Sigma^+$ states, and between the 3 and 4 $^1\Sigma^+$ states at $R \sim 12.70$ a.u. and 5.20 a.u., respectively, these couplings would affect the MN reaction cross section at higher energies.

Some important adiabatic rotational coupling matrix elements $A^{\theta}_{ij} = \langle \psi_i | \mathrm{i}L_y | \psi_j \rangle$ are shown in Fig. 2(b). These couplings drive the transitions between states with the same spin but different spatial symmetries. Due to strong adiabatic interactions between adjacent states, the rotational coupling near avoided crossings is not smooth, such as 4 $^1\Sigma^+$–2 $^1\Pi$ and 5 $^1\Sigma^+$–2 $^1\Pi$ at $R \sim 34.20$ a.u. In the non-adiabatic representation, these rotational coupling matrix elements become smooth.

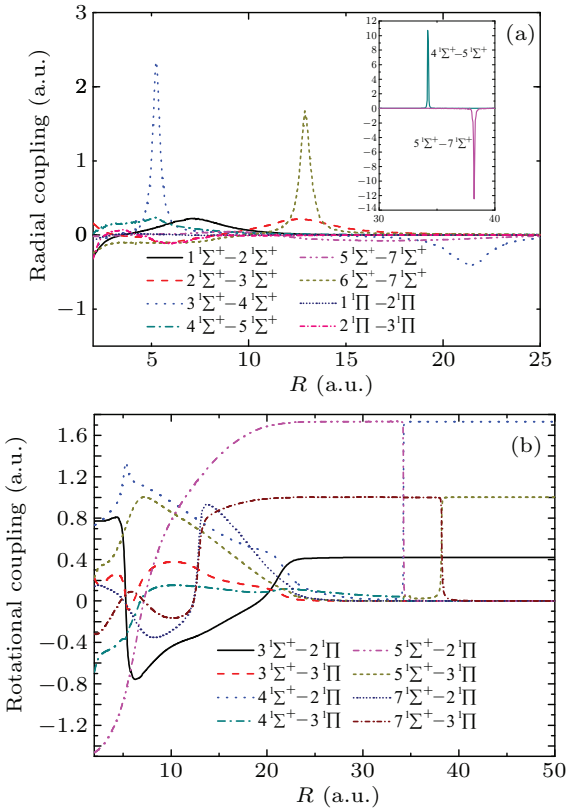


Fig. 2. Coupling matrix elements for NaH molecule: (a) radial coupling matrix elements and (b) rotational coupling matrix elements.

3. Result and discussion

In the present work, the low-energy mutual neutralization (MN) reaction of $Na^+ + H^-$ has been studied using the QMOCC method, which has been mentioned in our previous works.[27,28] In Fig. 3, the total charge-transfer cross sections of $Na^+ + H^-$ MN reactions are presented and compared with other theoretical results over a wide energy range of 10^{-3}–10^3 eV/u.[9–12]

For energies below 1 eV/u, the scattering cross section for the MN reaction is very large (greater than 10^{-13} cm^2), and it increases steeply as the energy decreases, reaching approximately 3.6×10^{-11} cm^2 at 10^{-3} eV/u. In comparison with other theoretical results, our results are in general agreement with all other theoretical results[10–12] in both magnitude and trend, and are in better agreement with the results of Dickinson *et al.*[9] due to the fact that the dynamical part of both calculations uses fully quantum (FQ) methods.

Moreover, for energies above 10 eV/u, the present MN total cross section shows a slow decreasing trend as the energy increases, the cross section is about 2.8×10^{-14} cm^2 and 2.2×10^{-14} cm^2 for the collision energy of around 10 eV/u and 10^3 eV/u, respectively. Similar properties of the scattering cross section are also observed in other MN reactions involving alkali positive Li^+, Cs^+ ions with H^- ions.[11,29,30] In contrast to our results, the calculated cross sections of Olson *et al.*[10] and Barklem *et al.*'s.[12] showed a significant decrease for energies above 10 eV/u based on the Landau–Zener dynamics with different methods for calculating the couplings, while at $E \sim 100$ eV/u, their cross section is approximately one-fifth of ours. The discrepancy may stem from two reasons: firstly, the LZ method only accounts for the most important avoided crossings and may not fully describe the MN collision reactions; secondly, Olson *et al.*[10] and Barklem *et al.*[12] may focused solely on the total cross sections of the final states of Na(4s, 3d, and 4p), for the non-LTE modeling of stellar atmospheres with the temperature below $\sim$ 10000 K (less than about 1 eV), and experimental and theoretical data indicate that the cross section of these three states accounts for over 99% of the total cross section at $E < 1$ eV/u.[7,9,29] To verify this conjecture, we also provided the total cross sections for the final states of Na(4s, 3d, and 4p) by using the QMOCC method, which are also shown as the dashed black line in Fig. 3. And the total cross section exhibits a similar trend of significant decrease with increasing collision energy as Olson *et al.*[10] and Barklem *et al.*[12]'s results. Therefore, the contributions from other excited states in addition to the (4s/3d/4p) states should be considered for energies above 10 eV/u.

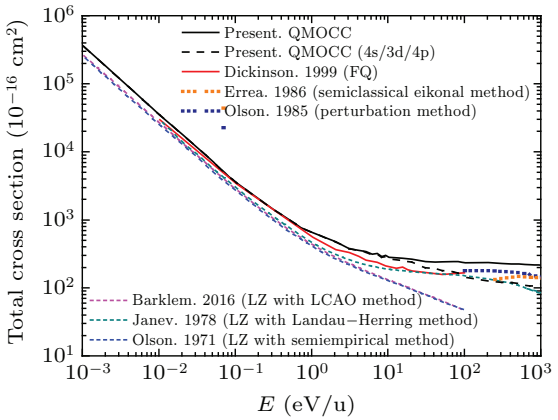


Fig. 3. Comparison between the present total cross sections with other theoretical results for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions. The theoretical results are from the present calculation of total cross sections (solid black line) and total cross sections for Na(4s/3d/4p) (dashed black line), quantum chemical results of Dickinson *et al.*[9] (solid red line), semiclassical result with a five-state molecular expansion of Errea *et al.*[14] (short dotted orange line), perturbation method of Olson *et al.*[13] (short dotted royal line), Landau–Zener model with LCAO method of Barklem *et al.*[12] (short dashed magenta line), Landau–Zener model with Landau–Herring method of Janev *et al.*[11] (short dashed dark cyan line), and Landau–Zener model with semiempirical (SE) couplings of Olson *et al.*[10] (short dashed blue line).

Furthermore, in the energy region above 10 eV/u, compared to the results obtained by Dickinson *et al.*[9] using the FQ method, our results are slightly larger, which may be introduced by the differences in structural calculations. In the present work, the influences of three $^1\Pi$ states and 10 active electrons are considered, while Dickinson *et al.*[9] only considered the outermost 2 active electrons and the influence of $^1\Pi$ state was not taken into account. Although the results of Janev *et al.*[11] for energies above 10 eV/u appear to be more consistent with Dickinson *et al.*'s,[9] but there may be some issues with it, which we can see from the part of states-elective cross section. Moreover, Errea *et al.*[14] and Olson *et al.*[13] also calculated the cross sections with the energy range of above 100 eV/u, but the excited states were not fully considered, some important states such as Na(3d and 4p) were not included in their calculations.

To further validate our results, in Fig. 4, the state-selective cross sections for the MN reactions of $Na^+ + H^- \rightarrow Na(nl) + H$ are presented. It can be seen that below 10 eV/u, the main reaction exit states for this process are the Na(4s and 3d) states, which are nearly more than one order of magnitude larger than other exit states. The Na(4s) is the most dominant state, the MN reaction cross section is about 2.8×10^{-11} cm^2 at $\sim 10^{-3}$ eV/u, and gradually decreases as the energy increases, and the cross section is about 1.9×10^{-14} cm^2 at $\sim$ 10 eV/u. The Na(3d) state is the secondary dominant exit state and has the same decreasing trend as the 4s state, but its magnitude is about a quarter of that of the 4s state. With the increase of energy, due to the competition between different states with the relatively complex radial and rotational coupling, the main final states of the scattering cross section for the MN reactions change. For example, it should be noted that the cross section of the Na(3p) state forms a valley around 1 eV/u, when the energy is above 100 eV/u, the dominant exit state becomes the Na(3p) state due to the strong and broad avoided crossing between the 2 and 3 $^1\Sigma^+$ states at $R \sim 12.70$ a.u., and the Na(3d) state becomes the secondary dominant exit state. This explains the slow decreasing trend observed of the MN total cross section in Fig. 3 for the energies above 10 eV/u. However, the Na(4s) state, which is the dominant exit state below 10 eV/u, becomes the third important exit state.

The magnitude of the state-selective cross sections in this MN reaction system is primarily determined by the interplay of two competing mechanisms. First, the cross sections vary inversely with energy, which is a result of the focusing effect of the Coulomb field.[9] The second component for the 3p and 3s states arises from the ionic-covalent interaction at relatively close internuclear distances (around $R \sim 13.00$ a.u. and 7.60 a.u., respectively), where avoided crossings exhibit a large adiabatic splitting. When the collision energy exceeds 1 eV/u, the cross sections increase with increasing en-

ergy. This behavior is also observed in other mutual neutralization processes, such as $Cs^+ + H^-$.[31] For the 5s, 4s, 3d and 4p states, the second contribution to the cross sections comes from the broad radial and rotational couplings as $R < 5.00$ a.u., which contribute to an increase of the cross sections in higher energy region. However, due to the cross sections of the 5s state being two orders of magnitude smaller than those of the 4s, 3d, and 4p states, the increase in cross sections of the 5s state appears more pronounced. It can be observed that for energies above 10 eV/u, some state-selective cross sections, such as 4s and 4p, exhibit relatively weak oscillatory structures. Such oscillatory structure may be interpreted as Stueckelberg oscillations, which can be explained as non-random phase contributions to the cross-section due to one or more extrema in the potential difference between the reactant and product states.[27]

The state-selective cross sections of the four most important exit states Na(3p, 4s, 3d, and 4p) for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions are also shown and compared with other theoretical[9,11,13,14] results in Fig. 5. It can be observed that, in the overlapping energy region, our results for the Na(3p, 4s, and 4p) exit states agree well with the results of Dickinson *et al.*[9] in both trend and magnitude. The main difference is the cross section of the Na(3d) exit state, particularly for energies above 10 eV/u, our calculated cross section is more than three times larger than theirs, which may be due to the differences in the structure calculations. When the energies are above 100 eV/u, our results for Na(4s and 3p) agree well with those of Errea *et al.*[14] and Olson *et al.*,[13] but it is a pity that the important exit states of Na(3d and 4p) were not considered in their works. However, although the results of Janev *et al.*[11] for the dominant exit state 4s are consistent with other theoretical results, there are significant differences in the numerical values of the other important Na(3p, 3d, and 4p) exit states. As their results differ greatly from the experimental data,[7] some inaccuracies may have been made in the calculations. In a word, new experimental measurements and theoretical data are expected, especially in the energy region above 10 eV/u.

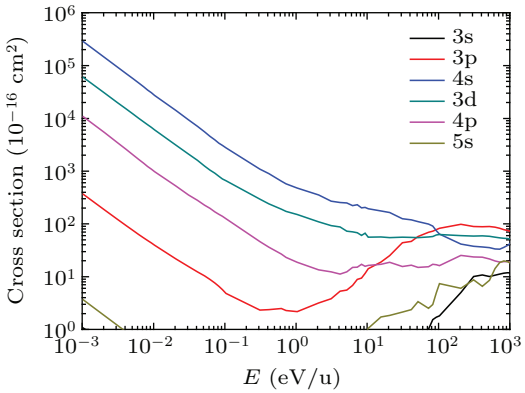


Fig. 4. The state-selective cross sections for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions.

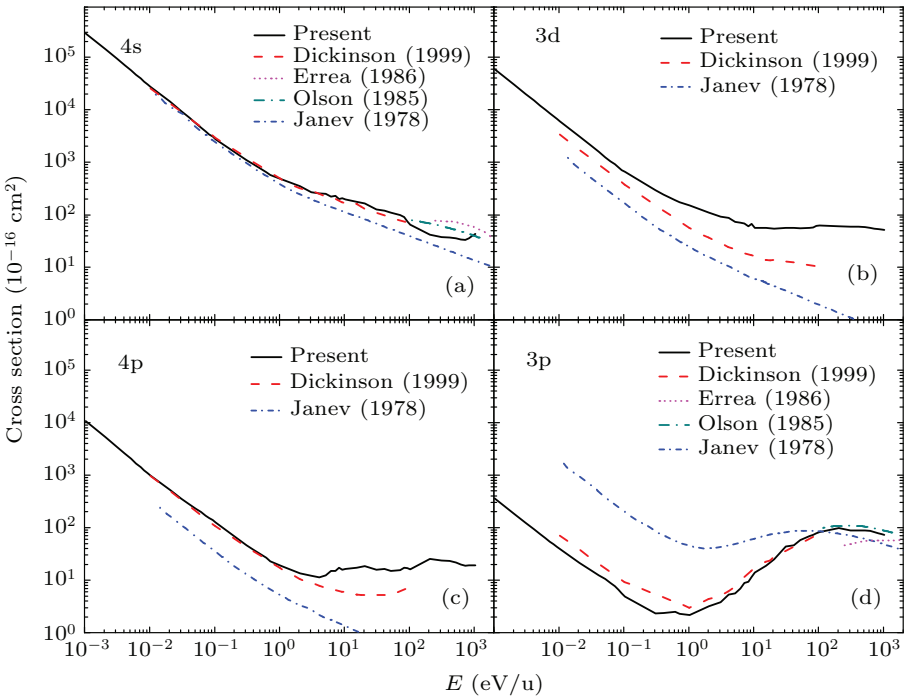


Fig. 5. Comparison of the state-selective cross sections with other theoretical[9,11,13,14] results for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions.

Up to now, only Eklund *et al.* have reported merged beam experiments on the mutual neutralization reactions of Na^+ and D^- at low energies, and have provided branch fractions for the cross sections of the primary exit states Na(4s, 3d, and 4p) for energies between 80 meV ($\sim$ 43 meV/u) and 393 meV ($\sim$ 214 meV/u),[7] and previous theoretical calculations have shown that the branch fractions of the cross sections of Na^+ with H^- and D^- ions are generally the same.[10,12] e.g., for the

dominant exit state Na(4s) in the energy range we considered, the error between the branch fractions of the cross sections with H^- and D^- ions is up to about 3%. Therefore, in Fig. 6, we show the branch fractions of the 4s, 3d, and 4p exit states by using the QMOCC method for the $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions, and compare them with other theoretical results.[9,10,12] It can be found that our results are in better agreement with the experimental data, especially for the dominant exit state Na(4s) in the MN reactions, contributing to $\sim 78\%$ for energy below 1 eV/u, and the branch fractions of 4s are all within the error bar of the experiment. In contrast, the branch fractions of the dominant exit state Na(4s) for the $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions are all above 85% in the energy region below 1 eV/u.

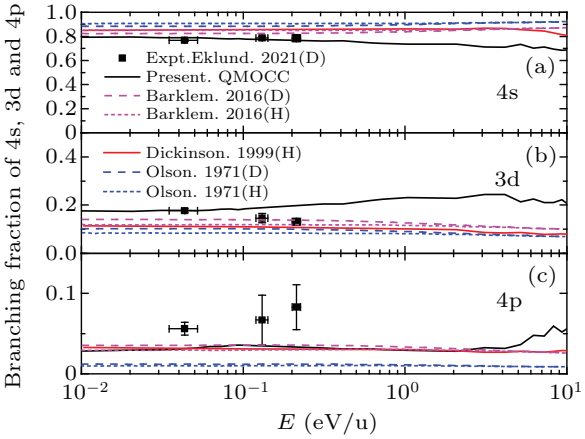


Fig. 6. Comparison between the present branching fraction of (a) 4s, (b) 3d and (c) 4p with other experimental[7] and theoretical[9,10,12] results for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions.

In order to facilitate the application of MN reactions in astrophysics, the state-selective rate coefficients have been investigated by averaging the scattering cross section using the Maxwellian–Boltzmann distribution. The resulting temperature-dependent reaction rate coefficient is given by the following formula:

$$\alpha(T) = \left(\frac{8}{\mu\pi}\right)^{1/2} \left(\frac{1}{kT}\right) \int_0^\infty E\sigma(E) \exp\left(-\frac{E}{kT}\right) \mathrm{d}E, \quad (2)$$

where k represents the Boltzmann constant, and μ represents the reduced mass. In Fig. 7, the state-selective rate coefficients for the temperature range of 100–10000 K are displayed. For the main exit states, the rate coefficients of the Na(4s, 3d, and 4p) exit states exhibit the same trend, slowly decreasing with increasing temperature. For example, for the dominant 4s state, the rate coefficient is on the order of 10^{-7} cm^3/s in the temperature range of 100–2000 K, and when the temperature increases to 10000 K, the rate coefficient decreases to about 7.62×10^{-8} cm^3/s. This result differs by no more than 5% in value from the theoretical calculation results of Barklem *et al.*[6]

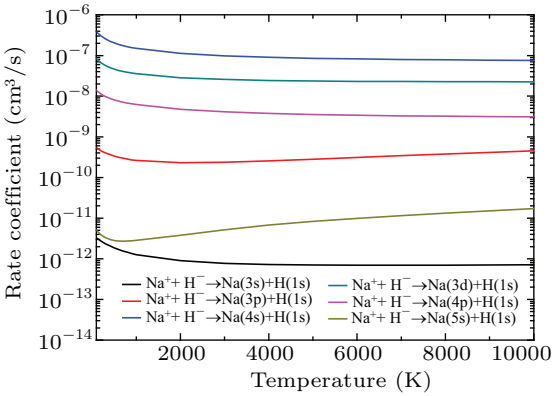


Fig. 7. The state-selective rate coefficient for $Na^+ + H^- \rightarrow Na(nl) + H$ MN reactions.

4. Conclusion

The low-energy mutual neutralization (MN) reaction between Na positive and H negative ions has significant importance in controlled fusion plasmas and astrophysics. In this work, the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method, which is the most reliable method for the low-energy collision, is used to study the MN reactions $Na^+ + H^- \rightarrow Na(nl) + H$ over a wide energy range from 10^{-3} eV/u to 10^3 eV/u, and this energy region covers the typical temperature conditions of many astrophysical and laboratory plasmas, including the edge plasmas of thermonuclear fusion devices.[8] The electronic structure parameters required for the dynamical calculations, including adiabatic potentials, radial and rotational coupling matrix elements, are calculated using the *ab initio* multi-reference single- and double-excitation configuration interaction (MRD-CI) method.[17,18]

The total and state-selective cross sections have been obtained and compared with the available theoretical[9–14] and experimental[7] results. For energies below 1 eV/u, our results are in general agreement with other theoretical ones that adopt the LZ method in both magnitude and trend, and are in better agreement with those of Dickinson *et al.*,[9] who used the fully quantum method. The dominant reaction exit states are the Na(4s, 3d, and 4p) states, among which the most important reaction state is the 4s state, and the contribution of branch fractions is about 78%. This result is currently the best match with experimental results.[7] For energies above 10 eV/u, the present MN total cross section is larger than those obtained in other theoretical calculations[9–14] and exhibits a slow decreasing trend. The main reason is that the primary exit state of the MN reaction changes due to the competition between different states with the relatively complex radial and rotational couplings. When the energy is above 100 eV/u, the dominant exit state becomes the Na(3p) state, while the Na(4s) state, which is the dominant exit state below 10 eV/u, becomes the third important exit state. New experimental measurements

are expected to verify it. Moreover, in order to facilitate the application of MN reactions in stellar atmosphere modeling, the state-selective rate coefficients have been investigated for the temperature range of 100–10000 K.

Data availability statement

The data that support the findings of this study are openly available in Science Data Bank via the link https://doi.org/10.57760/sciencedb.j00113.00112.

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