# §3. Charge Transfer in Collisions of $Si^{4+}$ Ions with He Atoms at Low-to-Intermediate Energies

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There have been three rigorous theoretical studies on electron capture in collisions of $Si^{4+}$ ions with He atoms at low energies below 10 eV/u [1]. Sizable discrepancies in rate coefficients calculated have been observed, and the origin of these discrepancies has remained unresolved. Therefore, we have carried out an *ab initio* theoretical investigation for electron capture in collisions of $Si^{4+}$ ions with He atoms at low collision energies and extended to much higher energy region up to 10 keV to shed some light on the problem as well as to understand the scattering dynamics at higher energies. The theoretical studies are based on a molecular orbital (MO) expansion method within a semiclassical formalism. The process we have studied is as follows, with corresponding asymptotic energy defects:

$Si^{4+}(2p^6)$+ He --->$Si^{3+}(3p)$ + $He^+$ -11.71 eV

--->$Si^{3+}(3s)$ + $He^+$- 20.55 eV.

In the present ab initio calculations, the AO basis set employed for the Si atom is (16s10p5d3f), contracted to [12s7p4d2f], augmented by two d and one f polarization functions. For the He atom, we employ the same basis set as was used before. The potential curves are obtained by the multireference single and double excitation (MRD-CI) configuration interaction method [2]. A semiclassical MO expansion method with a straight-line trajectory of the incident ion was employed to study the collision dynamics below 10 keV [3]. The total scattering wave function was expanded in terms of products of a molecular electronic state and atomic-type electron translation factors (ETFs) to satisfy the correct scattering boundary condition. Transitions between the molecular states are driven by nonadiabatic couplings. By solving the resulted first-order coupled equations in time t, we obtain the transition probabilities and hence, the scattering amplitudes in a standard procedure. Integration of the probability over the impact parameter gives the cross section. Adiabatic potentials for the $SiHe^{4+}$ system are shown in Fig.1 First two lowest leveles correspond to electron cvapture channels, followed by the ground [$Si^{4+}(2p^6)$ + He] initial channel. At higher above, there is a series of excited electron capture channels. Because of a curve crossing between the $3^1$_ and $2^1$_ states at R = 7.1 au, the radial coupling at this R plays a crucial role for dynamics, and hence, accurate description of the nonadiabatic coupling is essential.

References:

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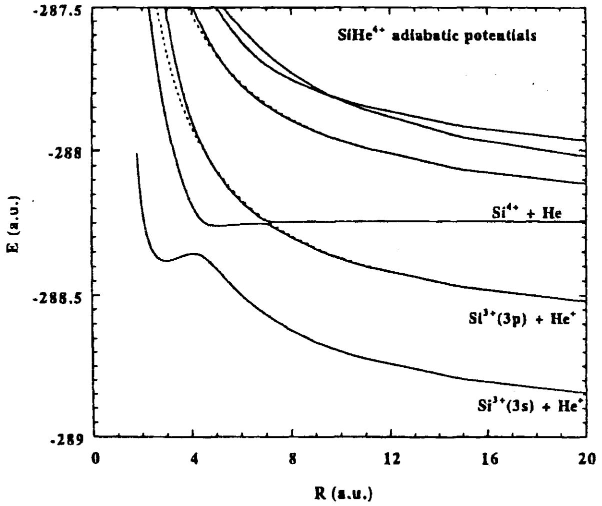

Fig. 1 Adiabatic potentials for the $SiHe^{4+}$.