AB INITIO STUDY OF CHARGE TRANSFER IN LOW ENERGY Si^{2+} COLLISIONS WITH ATOMIC HYDROGEN[1]

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Charge transfer cross sections for collisions of ground state $Si^{2+}(3s^2\ ^1S)$ and excited state $Si^{2+}(3s3p\ ^3P^o)$ with atomic hydrogen are presented for energies less than 100 eV/amu. The cross sections are calculated in a diabatic representation using a fully quantum-mechanical, molecular-orbital, close-coupled method. Completely *ab initio* adiabatic potentials and nonadiabatic radial coupling matrix elements obtained with the spin-coupled valence-bond method are incorporated. Inclusion of the $Si^{+}(3s3p^2\ ^2D) + H^{+}$ and $Si^{2+}(3s3p\ ^3P^o) + H(1s)$ closed-channels results in oscillations in the $Si^{2+}(3s^2\ ^1S)$ charge transfer cross section for collision energies above the separated-atom energy of the lowest closed-channel (~4.2 eV/amu). Rate coefficients for temperatures between 500 and 100 000 K and cross sections for collisions with isotopic D are presented. Results for the reverse process, charge transfer ionization, are also given.

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