Abstract Submitted
for the DAMOP05 Meeting of
The American Physical Society

Numerical study of charge transfer processes in collisions of Be^{4+} and He^{2+} with atomic hydrogen TATSUYA MINAMI, DAVID R. SCHULTZ, ORNL, MICHAEL S. PINDZOLA, Auburn University, TECK-GEE LEE, ORNL
— We have calculated state-selective charge-transfer cross sections in collisions of Be(4+ with H(1s) and of He^{2+} with H(1s). We have used the lattice time-dependent Schrödinger equation (LTDSE) approach, the atomic orbital coupled channel (AOCC) method, and the classical trajectory Monte Carlo (CTMC) method. The calculations are performed with impact energy ranging between 1keV/u and 1MeV/u. With a well chosen basis-function set, we have found that AOCC gives good agreement with LTDSE. Also, with regard to Wigner's n^{-3} law, we have found that CTMC gives good extrapolations to the cross sections calculated by LTDSE and AOCC toward high n levels such as for those greater than 6. Thus, in our presentation, we will propose theoretical values of the total charge-transfer cross sections for these collision systems based on a combination of the most reliable results of the various method. This research used resources of the Center for Computational Sciences at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC05-00OR22725, and also of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

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Date submitted: 28 Jan 2005 Electronic form version 1.4