Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Charge transfer in collision of H^+ with Li($1s^2 2s, 2p_z$): TD-MADNESS approach.[1] F. JAVIER DOMINGUEZ, PREDRAG S. KRSTIC, Stony Brook University — We study state-resolved charge transfer processes for H+ collisions with atomic neutral lithium, in its ground and first excited state, in range from 1 to 25 keV/amu. We solve numerically the time-dependent Schrodinger equation (TDSE), using TD-MADNESS, Time-Dependent version of the Multiresolution Adaptive Numerical Environment for Scientific Simulation [1]. An advantage of the MADNESS is that the desired local accuracy is input parameter to the calculation and the method adapts the multiresolution representation of the wavelets to obtain this accuracy. By working with the numerical mesh which adapts to the gradient of the potential, quite large numerical boxes can be used within realistic computing times. The large size numerical box in MADNESS enables accurate representations of the Rydberg states and continuum, usually a problem in other TDSE methods. The time evolution is modeled by the Chin-Chen representation of the evolution operator [2]. The atomic Li target is modeled by frozen-core pseudo-potential while the ion projectile follows a straight line trajectory. We report new benchmark data for charge transfer cross section to n=2, and 3 states of H from $1s^2 2s$ and $1s^2 2p_z$ of Li. Available theoretical and experimental data in the literature are in reasonable agreement with our results [3]. [1] R. J. Harrison et al., J. Chem. Phys. 121, 11587 (2004). [2] F. J. Dominguez et al., Adv. Quantum Chem. 71, 353 (2015) [3] F. J. Dominguez and P. S. Krstic, J. Phys. B 49, 195206 (2016).

[1]Research supported by CONACyT postdoctoral scholarship.

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Date submitted: 10 Nov 2016 Electronic form version 1.4