Abstract Submitted for the DAMOP16 Meeting of The American Physical Society

Stopping of Protons in Copper at low velocities^{*)} EDWIN E. QUASHIE, BIDHAN C. SAHA, Department of Physics, Florida A & M University, FL-32307., ALFREDO A. CORREA, Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, CA-94550 — An *ab initio* study including non-linear effects is reported of the electronic stopping power of protons in copper over a wide range of proton velocities (v = 0.01-10 a.u.). Time-dependent density functional theory coupled with molecular dynamics [1] is used to study electronic excitations produced by energetic protons. A plane-wave pseudo-potential scheme is employed to solve the time-dependent Kohn-Sham equations for a moving proton in a periodic copper crystal. These electronic excitations and the band structure determine the stopping power of the material and alter the interatomic forces for both channeling and off-channeling trajectories. Our off-channeling results are in quantitative agreement with experiments. Details will be presented at the conference [1] E. Runge and E. R. U. Gross, Phys. Rev. Lett. **52**, 997 (1984). *) Supported by NNSA

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