## Abstract Submitted for the DAMOP07 Meeting of The American Physical Society

Particle, Energy and Rovibrational Spectra of Molecules Chemically Sputtered of Carbon Surfaces<sup>1</sup> PREDRAG KRSTIC, CARLOS REIN-HOLD, Oak Ridge National Laboratory, STEVEN STUART, Clemson University — We perform classical molecular dynamics simulations of the chemical sputtering of deuterated amorphous carbon surfaces by deuterium atoms and molecules at impact energies from threshold to 50 eV/D. Particular attention is paid to the preparation of the target surfaces for varying impact projectile fluence, energy and species [1]. The spectra of hydrocarbon molecules  $C_xD_y$ , with x in range 1 to 5 are observed, and spectral distributions of their translational, rotational and vibrational energies are analyzed. Angular spectra of the sputtered molecules are also analyzed. Our results show good agreement with existing experimental data. [1] P. S. Krstic, C. O. Reinhold, and S. J. Stuart, Europhysics Letters 77, 33002(2007).

<sup>1</sup>We acknowledge support by the OFES (PSK) and the OBES (COR) of the U.S. DoE under contract No. DE-AC05-00OR22725 with UT-Battelle, LLC, and (SJS) of DoE (DE-FG02-01ER45889), the NSF (CHE-0239448) and a MURI managed by the ARO.

Predrag Krstic Oak Ridge National Laboratory

Date submitted: 06 Feb 2007 Electronic form version 1.4