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What Can We Learn on the Above-Surface Neutralization Process from the Chemical Sputtering Yields of D, D_2 AND D_3 at Carbon Surface?[1] PREDRAG S. KRSTIC, CARLOS C. REINHOLD, Oak Ridge National Laboratory, STEVEN J. STUART, Clemson University — We perform molecular dynamics simulations of chemical sputtering of methane and acetylene from deuterated amorphous carbon surface, by impact of deuterium, as well as of vibrationally excited D_2 and dissociating D_3 molecules in range of 5-30 eV/D impact energies. We show that the chemical sputtering yields at the lowest impact energies are very sensitive to the vibrational state of the molecules. Our sputtering yields are compared with those obtained experimentally [L.I. Vergara et al, J. Nucl. Mat. (2006), in press] by impact of D, D and D. Analyzing possible processes of the above-surface neutralization of the impinging ions in the experiment we conclude that the leading mechanism is the charge transfer from the surface-bound deuterium atoms onto vibrationally excited states of the molecules.

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Predrag S. Krstic
Oak Ridge National Laboratory

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