Elastic scattering of tritium and helium atoms on graphite surfaces: Potential energy function and quantum dynamical simulation

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We report simulations [1] of the elastic scattering of beams of tritium and helium atoms from graphite (0001) surfaces in an energy range of 1 to 4 eV. To this aim, we numerically solve a time-dependent Schrödinger equation using a split-step Fourier method. The tritium- and helium-graphite potentials are derived from density functional theory calculations using a cluster model for the graphite surface. We observe that the elastic interaction of tritium and helium with graphite differs fundamentally. Whereas the wave packets in the helium beam are directed to the centers of the aromatic cycles constituting the hexagonal graphite lattice, they are directed towards the rings in case of the tritium beam. These observations emphasize the importance of swift chemical sputtering for the chemical erosion of graphite and provide a fundamental justification of the graphite peeling mechanism observed in molecular dynamics studies. Our investigations imply that wave packet studies, complementary to classical atomistic molecular dynamics simulations open another angle to the microscopic view on the physics underlying the sputtering of graphite exposed to hot plasma.

[1] Stefan E. Huber, Tobias Hell, Michael Probst and Alexander Ostermann, Theoretical Chemistry Accounts 2013, in print