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First-principles reaction-path finding in gas discharge plasmas with QCEIMS REI SAKUMA, SATOSHI NAKAMURA, SHOGO SAKURAI, HIROYUKI KUBOTERA, KIYOSHI ISHIKAWA, ET Center, Samsung R&D Institute Japan, SUN-TAEK LIM, DAE SIN KIM, Semiconductor R&D Center, Samsung Electronics — Current plasma simulations for semiconductor plasma processes all rely on accurate reaction databases in gas discharges, but prediction of the reactions between discharged electrons and gas molecules remains a major theoretical challenge as these reactions involve complex electronic processes far beyond the scope of standard electronic-structure approaches. Aiming at constructing reliable reaction databases for plasma process simulations from first-principles, in this contribution we report an application of the recently-proposed reaction-path-finding program QCEIMS[1] for dissociative ionization of fluorocarbon gas molecules. QCEIMS is a molecular dynamics based approach which has been successful for reproducing experimental electron ionization mass spectra as well as describing dissociative electron attachment processes of several systems. As a first benchmark, we compute mass spectra of several fluorocarbon molecules and show that QCEIMS not only reproduces many of the major peaks of experimental mass spectra but also provides the corresponding trajectories, which makes it a promising tool for deducing dominant reaction pathways in plasma processes.

[1]S. Grimme, Angew. Chem., Int. Ed., 52, 6306 (2013); V. Ásgeirsson, C. A. Bauer, S. Grimme, Chem. Sci. 8, 4879 (2017).

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