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First principles simulations of molecules and nanostructures subjected to ion irradiation[1] KALMAN VARGA, SERGIY BUBIN, BIN WANG, SOKRATES PANTELIDES, Vanderbilt University — In the framework of real-time real-space time-dependent density functional theory complemented with classical molecular dynamics for ions, we have studied the behavior of small molecules and nanostructure fragments, such as graphene sheets, irradiated by charged energetic particles. In particular, we have investigated the importance of electronic excitations and examined the regime when bond breaking (or defect formation) occurs. Based on the microscopic description of these processes, several quantities that are of interest for ion beam physics have been determined, such as the amount of energy transferred to the target system and the distribution of this energy between electronic excitations and vibrational motion.

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