chem2Dmat
September 03-06, 2019 • Dresden, Germany
European Conference on Chemistry of Two-Dimensional Materials

MoS_2 monolayers under cluster ion irradiation: A molecular dynamics study

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Focused ion beams (FIB) have opened a new door on manipulation of low-dimensional materials and are sought to be particularly promising for patterning two-dimensional (2D) materials through tuning the energy, type, charge state of the incident particles and the supporting substrate [1,2,3]. This tool is recently employed to tackle the important issue of controlled pore creation in 2D materials to be performed as filters for water desalination, gas sensing, etc. This aim requires a clear insight into the microscopic process which is yet to be fully understood. In this work, we use classical Molecular Dynamics (MD) simulations to shed light on the behavior of 2D materials under cluster ion irradiation, and specifically focus on the production and characterization of defects. To a great extent, the properties of the induced defects depend on the size and energy of the clusters, which to our knowledge, has not been studied to irradiate beyond graphene so far [4]. In particular, we are focused on the response of MoS_2 monolayers, which have shown various exciting properties complementary to graphene, under cluster irradiation. Furthermore, we show that depending on the incident angle and energy of the clusters, sulfur atoms can be sputtered mainly from the top layer, creating unique opportunities for patterning MoS_2 monolayers.

References

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