# Molecular dynamics modelling of primary radiation damage in materials

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I will give a tutorial of molecular dynamics simulations, focusing on aspects most relevant to simulating primary radiation damage. I will present the molecular dynamics (MD) method in general, and then describe special features that are needed to make the MD method suitable for efficient simulations of irradiation effects. These include recipes how to add realistic high-energy potentials, include electronic stopping, and use an adaptive time step.

I will also describe MD simulations in the recoil interaction approximation (RIA), and how such simulations can be used to get a comprehensive view of ion channeling, as well as very recent experimental and simulations results on how the sputtering yields are strongly affected by channeling in tungsten.