

# **"Molecular dynamics for materials research: from ion trails to protein adsorption"**

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The technique of molecular-dynamics simulation offers a high potential for materials research, since it provides the user with atomistic insight into the processes occurring in the material. I will discuss several recent examples of its use with an emphasis on non-equilibrium situations.

- Trails induced by keV ions on surfaces
- Bond breaking and reformation in swift-heavy-ion induced tracks:
  - \* strand breaks of DNA in cancer therapy
  - \* chemical processes in astrophysical ices
- Protein adsorption and pull-off: use of accelerated molecular dynamics

These examples allow us to discuss the potentials and pitfalls of atomistic simulation in novel applications.