Materials simulations from first principles and Molecular Dynamics with application in the fusion R&D

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Developing commercially viable fusion power plants depends crucially on finding materials that can tolerate the extreme reactor conditions. Most of the particularly crucial materials challenges start from atomic-scale processes, such as radiation damage, sputtering, diffusion, and creep. Hence reliable description of atom-level processes is crucial to tackle the fusion materials physics. This far the materials research was relying on analytical descriptions of interatomic interactions, so-called interatomic potentials, that are developed based on classical considerations of interatomic interactions to fit to specific properties of the material. Although usually quite efficient, these potentials frequently fail to describe consistently the properties of materials. During the last decade, machine learning approaches based on a systematic training against quantum mechanical (first principles) database have emerged as an interesting alternative. While showing impressive results for equilibrium and near-equilibrium materials properties, they have to date not been suitable for describing the far from equilibrium conditions that occur in the fusion reactor radiation environment.

In this talk, I will describe how we extended the Gaussian approximation machine learned potentials with a systematic fit to high-energy repulsive pair potentials, to enable a fully first-principles based approach to model atom-level materials effects both in near and far from equilibrium conditions. I will present examples of GAP potentials developed for both pure metals and complex alloys, and in particular the tabulated GAP (tabGAP) formalism that allows for an efficient description of multielemental alloys. I will then give examples of how this approach can be used for modelling radiation damage, elemental segregation and sputtering in materials of interest for fusion power plants.