Extending ab initio plasma-surface simulations to experimentally relevant scales

MICHAEL BONITZ, ALEXEY FILINOV, Univ Kiel, DETLEF LOFFHAGEN, INP Greifswald — Reliable and predictive plasma-surface modeling is crucial, both, for fundamental understanding and for many applications of low-temperature plasmas. The available approaches comprise phenomenological models of different complexity and quality as well as ab initio approaches that include density functional theory, quantum kinetic theory and molecular dynamics, for an overview see [1]. While the former suffer from a lack of reliable input parameters, the latter often are reliable but extremely time consuming and are, therefore, typically, applicable only to very short times and/or system size. Here I present a general concept how the ab initio methods can be extended, both, in length and simulation time. The idea is to properly combine ab initio simulations with lower level models [2]. I discuss how and when this can be done rigorously and present some examples [2, 3].