Towards the Simulation of Plasma Chemistries from Atomistic and Molecular First Principles Methods

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ABSTRACT

Ab initio quantum chemistry (AIQC) techniques and classical molecular dynamics based on AIQC are proposed to be used in a concerted manner to understand the physics and chemistry of plasmas. The computational approach consists of the traditional AIQC levels of theory for the calculation of finite and extended systems plus the use of modern density functional methods (DFT) and time-dependent DFT (TD-DFT), which in turn provide parameters and inputs for the development of mesoscopic methods of electron transport and nuclei classical molecular dynamics. The combination of these later two procedures is proposed for a realistic and computationally effective analysis of plasmas. An effective use of the above methods in a bottom-up approach has been developed for the in-progress study of non-plasmatic systems, such as a nanobattery, and preliminary calculations are being performed on plasmatic systems, leading to the simulation of a nano-fusion reactor, which eventually will provide useful atomic and molecular (A&M) data for fusion edge plasma transport in order to improve the development of materials supporting high flux heat and neutron activation. A major contribution of this work would be the study of matter interphases created at the edges of the plasma.

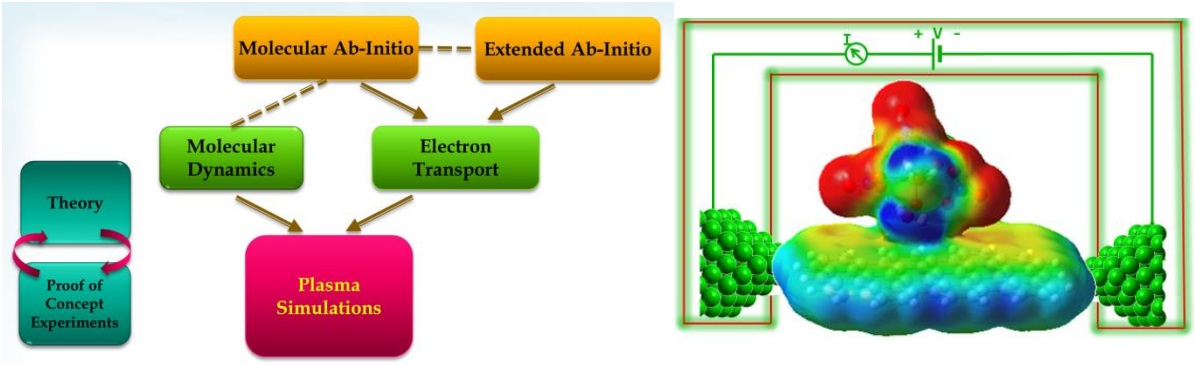

Figure 1. Left: Block diagram of the approaches combined together to determine properties and characteristics of materials, especially at interphases. Right: Cartoon showing the bottom-up approach to determine electron transport (ET) effects of electric fields through A&M systems [1-16].

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