Helium-based plasma interactions with air molecules

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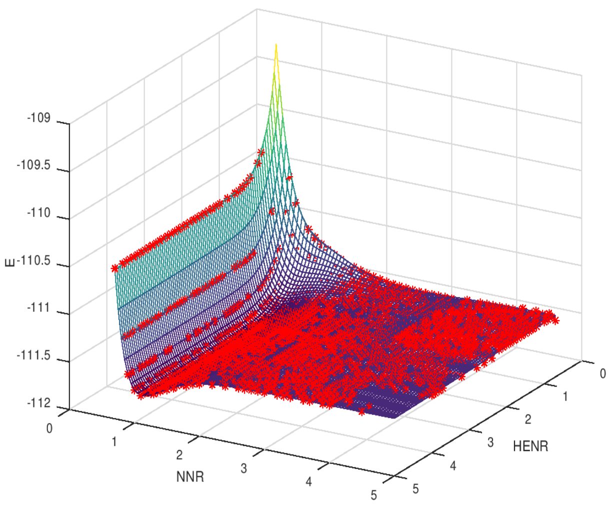
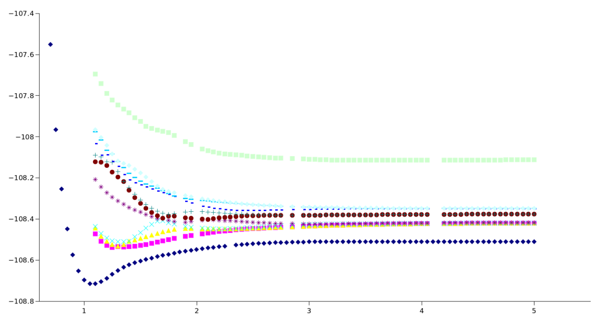
Résumé

Modeling of cold rare-gas plasmas is currently one of the popular topics in the field of quantum chemistry because of their possible applications in many other fields, e.g. surface treatment [1], food industry [2] or plasma medicine [3], with the last being the most interesting to our team. It was shown previously that rare-gas plasmas are well-working in such applications, which resulted in broad research in this field [4]. To understand the healing properties of cold rare-gas plasmas, detailed knowledge of processes on the microscopic level is of crucial importance. This talk will be focused on interactions between rare-gas ions and air molecules with the main focus on the simplest rare-gas (He) and the most abundant air molecule (N2). However, both the ab initio computations of potential energy surfaces and the semiclassical nonadiabatic molecular dynamics are very computationally demanding and, in some cases, even the modern computation methods show themselves unstable. The one way to overcome these obstacles is the utilization of machine learning methods, especially artificial neural networks (ANNs). Thus, this talk is going to cover our work both in ab initio computations of potential energy surfaces and their ANN representations.





Références

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