
ZAJEDNIČKI KOLOKVIJ
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Quantum wave packet method for 4-atom reactions: AB + CD R ABC + D

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Understanding dynamics of collisions at molecular level is the key to understanding reactivity. Theoretical treatment of molecular collisions relies on the calculation of the nuclear interaction potential and the motion of nuclei, governed by their electron clouds.

Exact quantum-mechanical treatments of nuclear motion on ab initio potentials have recently yielded remarkable agreements between theory and experiment for smallest 3-atom systems. Motivated by this success, we have been developing an exact time-dependent method for treating nuclear motion in 4-atom systems.

I will present the challenges we face in those calculations, such as exponential scaling and the notorious "coordinate problem", and how we deal with them in our methodology. I will describe our recent work in which we test the method on the H2 + OH R H2O + H reaction and the progress towards an ab initio calculation of the fully resolved angular product distributions in this 6-dimensional quantum system.

http://www.sid.cam.ac.uk/people/person.html?crsid=mtc34

voditelji seminara H. Buljan (FO) & B. Horvatić i M. Kralj (IF)