

A
FIZIKAI INTÉZET
és az
ATOMKI
közös
SZEMINÁRIUMA

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Diabatic Strategies for Molecular Photodynamics

címmel előadást tart

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szerdán
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az

MTA Atommagkutató Intézet

VIII. épület, 2. szemináriumi teremben (II.em. 202)

Short abstract: This presentation will address how a diabatic representation may provide a practical framework for simulating nonadiabatic processes with quantum dynamics, either with grid-based or on-the-fly Gaussian-based methods, but also for rationalising photoinduced mechanisms. This will be illustrated with some selected test cases showing interesting photochemical or photophysical properties.

