CFEL SCIENCE

SEMINAR

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CFEL-bldg. 99, seminar room IV

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System-bath quantum dynamics for energy transfer at surfaces

In non-equilibrium quantum dynamics, often an atom or molecule (the “system”) is embedded in an environment (or “bath”), which gives rise to energy and phase relaxation. This affects the spectroscopic response of the system, its reactivity, and its dynamics in general.

In this talk I will mostly consider the special case of vibrationally excited atoms or molecules at solid surfaces, which play a role in surface spectroscopy and surface photochemistry. Here we focus on fundamental aspects of energy and phase relaxation by adsorbate-phonon (for all surfaces) and / or adsorbate-electron / hole pair coupling (for metal surfaces). A “system plus bath” approach to multidimensional quantum dynamics will be followed, treated either by a multidimensional time-dependent Schrödinger equation (using, for example, the Multi Configurational Time Dependent Hartree (MCTDH) method [1,2,3,4] or an “exactly” solvable, so called Bixon-Jortner model [5]), or by a reduced description in which an open-system Liouville von Neumann is solved [2,3,6], instead. Issues of Markovianity, finite temperature effects, spectroscopy, and optical controllability of / in open systems will be addressed. Besides model problems [2,3,4], the concrete examples of energy and phase relaxation at H-covered silicon [1,5,7,8,9] and CO-covered copper surfaces[6] will be considered.

References:

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Host: Robin Santra – CFEL-DESY Theory Division