Real-space nonequilibrium dynamical-mean simulations for photo-excited hetero-structures and surfaces

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Using time-resolved pump-probe spectroscopies, one can probe the dynamics of correlated systems on femtosecond timescales, which allows to track the motion of electrons on the timescale of the hopping. A fascinating new development in these experiments is the investigation of correlated hetero-structures, which combines advances in material design and ultra-fast control. The nonequilibrium extension of dynamical mean-field theory (DMFT) has the potential to theoretically describe correlated systems out of equilibrium and make predictions for time-resolved optical and photoemission spectroscopy.
We have extended the nonequilibrium DMFT formalism to layered inhomogeneous
systems by adapting the real-space DMFT method to Keldysh Green functions [1].
Solving the resulting coupled impurity problems by means of the strong-coupling
perturbation theory, we apply the formalism to study the spreading of photo-excited
carriers from the surface of a hetero-structure into a Mott insulating bulk, and the induced changes of the electronic properties with time and space resolution.

[1] M. Eckstein and Ph. Werner, Phys. Rev. B 88, 075135 (2013).