

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Photoexcitations in a 1D manganite model: From quasiclassical light absorption to quasiparticle relaxations**<sup>1</sup> T. KÖHLER, O. SCHUMANN, F. BIEBL, S. KRAMER, S. KEHREIN, S. MANMANA, Inst. f. Theo. Phys., U. Göttingen, Germany, S. RAJPUROHIT, M. SOTOUDEH, P. BLÖCHL, Inst. f. Theo. Phys., TU Clausthal, Germany — We investigate 1D correlated systems following a photoexcitation by combining ab-initio methods, time-dependent matrix product state (MPS) approaches, analytical insights from linearized quantum Boltzmann equations (LBE), and molecular dynamics (MD) simulations to describe the dynamics on different time scales ranging from femto- up to nanoseconds. This is done for manganite systems in the material class  $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$ . We derive 1D ab-initio model Hamiltonians for which we compute the ground states at different values of the doping using MD simulations. At half doping, we obtain a magnetic microstructure of alternating dimers from which we derive a 1D Hubbard-type model. The dynamics is analyzed concerning the formation and lifetime of such quasiparticles via a LBE. We find that the magnetic microstructure strongly enhances the lifetime of the excitations. In this way, our work constitutes a first step to building a unifying theoretical framework for the description of photoexcitations in strongly correlated materials over a wide range of time scales, capable of making predictions for ongoing experiments investigating pump-probe situations and unconventional photovoltaics.

<sup>1</sup>Financial support from the Deutsche Forschungsgemeinschaft (DFG) through SFB/CRC1073 (Projects B03 and C03) is gratefully acknowledged.

Thomas Köhler  
Inst. f. Theo. Phys., U. Göttingen, Germany

Date submitted: 10 Nov 2016

Electronic form version 1.4