Simulations of Photo-induced Non-Equilibrium Dynamics in Charge Density Wave Materials

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We present the results of our computational simulations for non-equilibrium dynamic, obtained by computational resources at IST ARCS in NJIT. Our simulations focus on the non-equilibrium dynamic of distortion of crystal structure and electronic states, initiated by optical pulses, in a class of materials known as “charge density wave materials”. We use coupled Newtonian equations and the Boltzmann equations to simulate the time-evolution of our model system. We find that the high computing power at ARCS has been essential for us to obtain physically meaningful results.

This work has been done in collaboration with T. F. Seman and M. van Veenendaal at Argonne National Laboratory.