

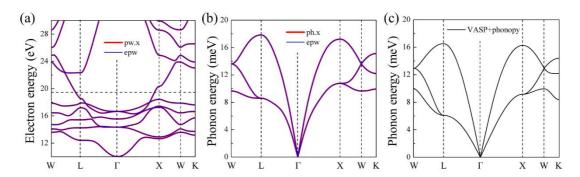
# Supplementary information

Out-of-equilibrium ultrafast electron and phonon energy transfer dynamics in metals: The role of non-thermal effect

Gui-Lin Zhu, Jing-Tao Lü

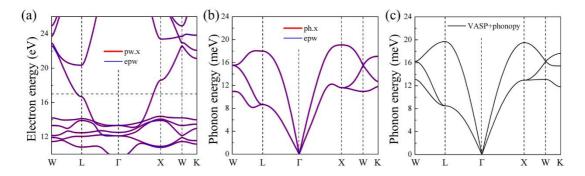
#### 1. The validation of Wannierization

#### 1.1 Electronic and phononic band structures of gold



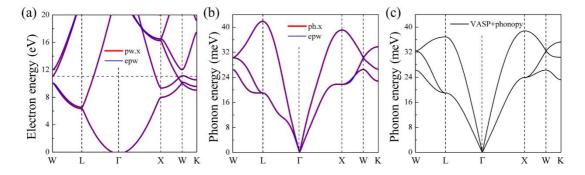
**Figure S1.** (a) Electronic and (b-c) phononic band structures of gold calculated by DFT and their Wannier interpolation. The horizontal dashed line in (a) represents the Fermi energy.

#### 1.2 Electronic and phononic band structures of silver



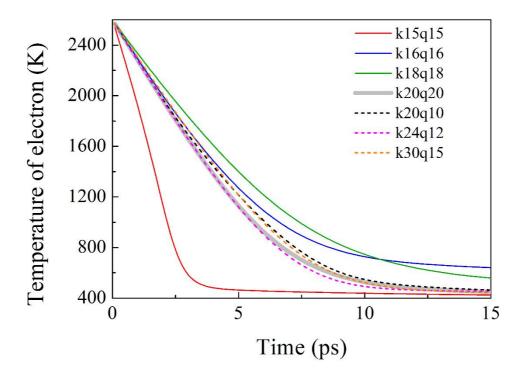
**Figure S2.** (a) Electronic and (b-c) phononic band structures of silver calculated by DFT and their Wannier interpolation. The horizontal dashed line in (a) represents the Fermi energy.

#### 1.3 Electronic and phononic band structures of aluminum



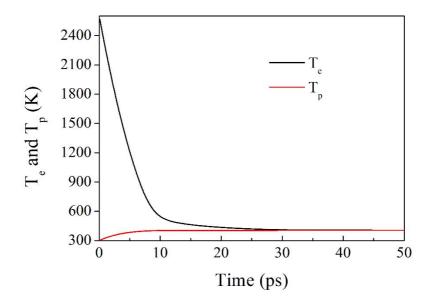
**Figure S3.** (a) Electronic and (b-c) phononic band structures of aluminum calculated by DFT and their Wannier interpolation. The horizontal dashed line in (a) represents the Fermi energy.

### 2. The convergence of the relaxation dynamic with k-/q- grid in gold



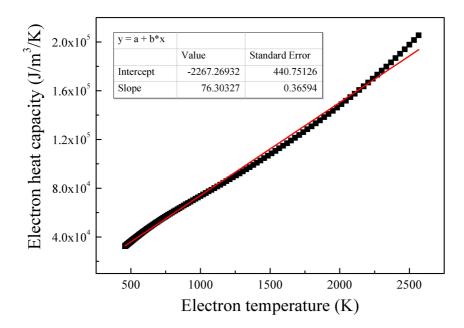
**Figure S4.** Electron temperatures during relaxation with  $\tau_{e^-e}$  = 40 fs, from 0 to 15 ps in gold. For example, k20q10 means that the k-mesh and q-mesh density is 20 × 20 × 20 grid and 10 × 10 grid, respectively.

#### 3. Long-time out-of-equilibrium dynamics in gold



**Figure S5.** Electron (black line) and phonon (red line) temperature during relaxation with  $\tau_{e-e}$  = 40 fs, from 0 to 50 ps in gold.

## 4. The electron heat capacity in gold



**Figure S6.** Electron heat capacity as a function of the electron temperature ( $T_e$ ) in gold. The electron specific heat constant is determined as the slope of a linear fit.