This is an example of calculation of the electronic heat capacity in multiple materials XTANT-3 code[[1]](#footnote-1).

In this example, it is assumed that you use the standard input files with material parameters provided with the code, including all the materials to be calculated. Multiple input files will be created at the code run, using the parameters from the file Copy\_input.txt (see manual for details).

1. Place both files, INPUT.txt and Copy\_input.txt into the directory INPUT\_DATA. The first file contains an example of calculation of the electronic heat capacity (without running the molecular dynamics, only using the TB for electron-phonon heat conductivity calculations, and MC for electron-electron contribution). The second file contains the instructions to create copies of the input files, replacing only the lines specified in this file.
2. Compile the code by calling Make.exe (under Windows) or make (under Unix).
3. Run the compiled code XTANT.exe or XTANT.x. It will create output directory with all the output files and plots created with gnuplot (if it is installed in your computer and the paths to it are set in the system). After calculations for one material, the next will start automatically, following the list specified in the Copy\_input.txt file.

1. <https://github.com/N-Medvedev/XTANT-3> [↑](#footnote-ref-1)