

2002 Summer School on Computational Material Science

Lab exercise on the code TBGreen – Umberto Ravaioli

TBGreen is the demonstration version of a more general code to evaluate the transmission and reflection coefficients for electron modes in a 2-D electron wave-guide structure, using a recursive Green's function approach as discussed in the lecture. This version is resident on the nanoHUB of the PUNCH system at Purdue University and it is limited to the calculation of the results for the first mode. A full version of the code may be obtained from U. Ravaioli. After login at the nanoHUB (<http://www.nanohub.purdue.edu>), click on the TBGreen button. You will reach the following interface:



[Hub Directory](#)

User: ravaioli | Run TBGreen. [Help](#) Available.

TBGreen-Related Information

[Description](#)

[Manual](#)

[Questions](#)

[Forum](#)

[Run Status](#)

Run TBGreen

1. [Modify/Create TBGreen Input Files](#)
 2. [Execute TBGreen](#)
 3. [View/Download TBGreen Output Files](#)
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Nanotechnology Simulation Hub

[PUNCH User's Manual](#) | [PUNCH-Related Questions/Comments](#)

Review the “Manual” link for information on the code, and for a sample input file. The input file is created or uploaded through link “1. Modify/Create TBGreen Input Files”. Then, click on “Execute TBGreen” to run the code. Directions on the web site are self-explanatory.