

## ENGINEERING/TECHNOLOGY

### Online Simulation Tools for Thermoelectric Energy Conversion Materials and Devices on nanoHUB.org

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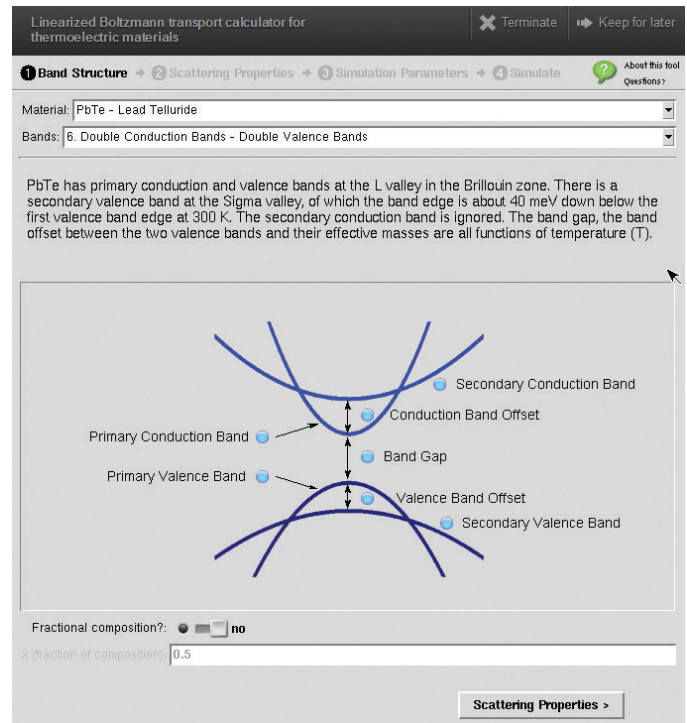
Advancement of technology allows the distribution of education around the world. In 2002, nanoHUB.org was launched for this very purpose. Since its launch, nanoHUB.org has successfully converted large amounts of complex research-based knowledge into simple online simulation tools. This eliminates the need of sophisticated hardware and expensive software to conduct various simulations.

Recently, a tool was launched on nanoHUB.org with the goal to teach thermoelectric energy conversion transport physics and its applications. With its simple and easy-to-use graphical user interface (GUI), this tool is packed with simulators based on the codes that are used in recent research papers. The first simulator, BTE Solver (<http://nanohub.org/tools/btesolver>), allows optimization of material properties to increase efficiency of thermoelectric energy conversion. The simulation is based on the modeling of electron transport, as well as electron-heat interactions inside the material according to the Boltzmann transport equation. The second simulator, TE Device (<http://nanohub.org/tools/teDEV>), allows users to optimize performance of thermoelectric energy conversion devices by comparing the system efficiency and the cost related to the process.

These two simulators were made using the latest version of the Rapture (Rapid Application Infrastructure) developers' toolkit by the Network for Computational Nanotechnology, which allows easy usage of the simulators. Entering device parameters through fields is minimized by replacing most input parameters with interactive images. This allows users with different computational skills to utilize the tool easily.

The tool was first featured in an online nanoHUB-U course, "Thermoelectricity: From Atoms to Systems" (<https://nanohub.org/courses/TEAS>) and received very positive feedback from students. It has helped students deepen their understanding of thermoelectric materials and systems.

*Research advisor Ali Shakouri and postdoctoral research associate Je-Hyeong Bahk write, "Kevin worked with great enthusiasm and creativity to develop an intuitive and easy-to-use graphical user interface for sophisticated online simulation tools that are based on the latest research results. His contribution greatly helped users to better understand the principles of direct thermal to electric energy conversion technologies."*



BTE Solver graphical user interface GUI.

Margatan, K. (2014). Online simulation tools for thermoelectric energy conversion materials and devices on nanoHUB.org. *Journal of Purdue Undergraduate Research*, 4, 80–81. <http://dx.doi.org/10.5703/1288284315445>