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Electronic structure modeling in an engineering context

Clint B Geller

Bechtel Bettis Laboratory, West Mifflin, PA 15134, USA

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Abstract
From 1994 through 2005 the US Department of Energy developed advanced thermophotovoltaic devices with world record energy conversion efficiency. I discuss my role as a materials physicist and electronic structure modeler embedded in this engineering development effort, in which I supported device design improvements throughout the project. I then generalize from these and other experiences to discuss the critical interfaces needed between potential electronic structure tool users in engineering organizations in industry and government, and electronic structure tool developers in academia.

