

Computational nanoelectronics is an emerging multi-disciplinary field covering condensed matter physics, applied mathematics, computer science, and electronic engineering. In recent decades, a few state-of-the-art software packages have been developed to carry out first-principle atomistic device simulations. Nevertheless those packages are either black boxes (commercial codes) or accessible only to very limited users (private research codes). The purpose of this book is to open one of the commercial black boxes, and to demonstrate the complete procedure from theoretical derivation, to numerical implementation, all the way to device simulation. Meanwhile the affiliated source code constitutes an open platform for new researchers. This is the first book of its kind. We hope the book will make a modest contribution to the field of computational nanoelectronics.

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