Abstract Submission Template

-Instructions- PLEASE READ

1. Do not alter this template.
2. Anything typed outside the "Replace this text with your abstract title/body" area will be ignored.
3. For scientific equations, use only standard characters, Microsoft Equations Objects, or MathType.
4. If you wish to embed a webpage, use the "Insert Hyperlink" function within Microsoft Word.
5. Do not insert Charts or Images into the abstract. This will cause your abstract to be rejected after submission.
6. Do not retype author lists. These will be automatically added; add only your abstract in between the "abstract" delimiters and your title in between the "title" delimiters.
7. Do not alter the fonts or size/color of the text. Such changes will be ignored and replaced with the standard.
8. There is a limit of 1300 characters. However, depending on such variables as the amount of "white space" or use of mathematical equations, some abstracts with less than 1300 characters will exceed our publication space limitations, and will be rejected. You will be able to preview your formatted abstract and check its length later in the submission process.
9. When saving this document. Use "File -> Save AS' and save as an RTF document. Please note the location where you save this document as you will need it when you upload it using the browse button.

-/Instructions-

-title-

Thermoelectric Properties of Ultra Narrow Silicon Nanowires from Atomistic Calculations

-/title-

-abstract-

The progress in nanomaterials' synthesis allows the realization of thermoelectric devices based on 1D nanowires (NWs). In these confined systems the electrical and thermal conductivities, and the Seebeck coefficient can be designed to some degree independently, providing enhanced ZT values as compared to the bulk material's value. We calculate the electrical conductivity, the Seebeck coefficient, and the electronic part of the thermal conductivity of scaled Si NWs. We use the atomistic sp3d5s*-spin-orbit-coupled tight-binding model and linearized Boltzmann transport. Our calculations include up to 5500 atoms, a task still computationally affordable within this model. We examine n-type and p-type NWs of diameters between 3nm and 12nm for [100], [110] and [111] transport orientations, at different doping levels. Using experimentally measured values for the lattice thermal conductivity, the expected ZT values of the nanowires are estimated. We further provide directions for power factor optimization with structure confinement.

-/abstract-