Dear Sir/Madam,

We are submitting the manuscript entitled “Ultrathin GaN Nanowires: Electronic, Thermal, and Thermoelectric Properties,” by A. H. Davoody, E. B. Ramayya, L. N. Maurer, and I. Knezevic, for publication in Physical Review B.

In recent decades, many efforts have been done to develop high efficiency thermoelectric (TE) devices. Highly doped semiconductors are known to be the materials with the highest TE figure of merit (ZT) by providing separate pathways for electrical and thermal transport. Moreover, thermoelectric figure of merit could be enhanced by employing nanostructured materials owing to the modified density-of-states and quenched thermal transport in such materials. Using TE devices for the purpose of energy harvesting requires materials with high TE figure of merit and thermal stability at high temperatures, and chemical stability in oxide environment. Bulk GaN has good thermal and chemical stability however it has been reported that its thermoelectric efficiency is relatively poor (ZT = 0.0017 at 300 K and 0.07 at 1000 K, as reported by Liu and Balandin). Here, we theoretically investigate how well nanostructuring, in particular using nanowires (NWs), can improve TE figure of merit in GaN-based TE devices.

In this paper, the suitability of using rough GaN NWs for high-temperature TE applications is theoretically investigated. We simulate electrical and thermal and TE properties of GaN NWs over a wide range of thickness (3-9 nm), doping densities (1018-1020 cm-3), and temperatures (300-1000 K). We use ensemble Monte Carlo technique coupled with a self-consistent Schrodinger-Poisson solver to simulate electronic transport. The electronic Seebeck coefficient and thermal conductivity is calculated by solving Boltzmann transport equation under relaxation time approximation. Lattice thermal conductivity is calculated based on a phonon ensemble Monte Carlo simulation, with a real-space realization of the rough surfaces. For the entire, temperature range, the Seebeck coefficient increases while the lattice thermal conductivity decreases with decreasing wire cross section. At room temperature these benefits are eventually overcome by the detrimental effect of surface roughness scattering on the electron mobility, so the peak ZT=0.2 is achieved at 4 nm. At 1000 K, the electron mobility is relatively flat due to the dominance of polar optical phonon scattering and contribution of multiple subband in transport. As a result, ZT keeps increasing with reducing wire thickness down to 3 nm. A peak value of ZT=0.8 is calculated for such NWs. The effect of doping density is shown to be important in producing a device with highest possible efficiency. For small 4 nm NWs the optimum doping density is found to be at 2\*1019 cm-3. Finally, an increase by a factor of 2 enhancement in ZT is observed when the temperature is increased from 300 K to 1000 K.

We believe that the work will be of interest to a broad range of scientists who work in the presently very active field of nanostructures thermoelectrics.

Thank you for your consideration,

Yours sincerely,