

Research Internship for 2020-21



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Theoretical study of thermoelectric properties beyond the linear response of Single Electron Transistor

Scientific Context

Specific properties of nanostructures have generated a recent revival of interest in thermoelectric devices [1]. Thanks to their delta-like density of states, devices based on quantum dots are expected to exhibit high Seebeck coefficient, nearly zero electronic thermal conductance and ultra-low phononic thermal conductance if embedded in an oxide matrix [2]. Due to single-electron tunneling across discrete levels in the Quantum Dot (QD), such devices are likely to behave as quasi-ideal energy filters giving rise to **incomparable thermoelectric properties, i.e. with an efficiency very close to the ideal Carnot efficiency**. An internship position dedicated to the simulation of such device is available in the **COMputational electronICS group** belonging to Center of Nanosciences and Nanostructures.

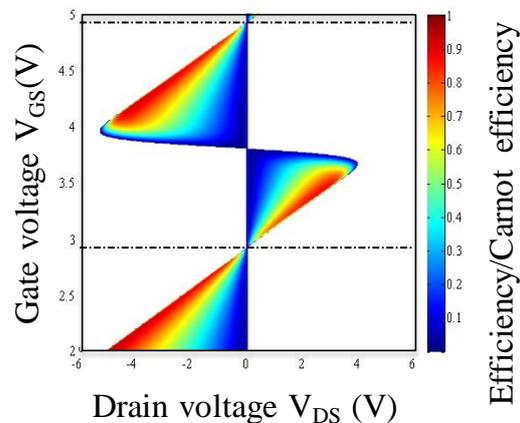
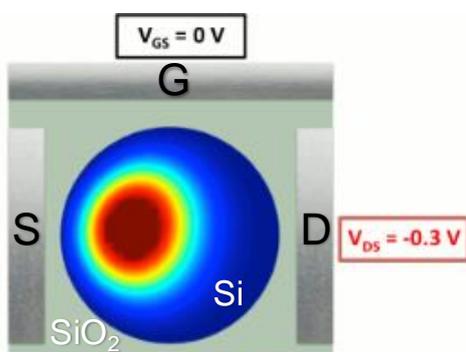


Fig. 1: Schema of a Single electron transistor (SET) with a map of electron density for one electron in the QD. Fig. 2: Cartography of normalized conversion efficiency.

Methodology and objectives

By using our homemade code consisting in a 3D Poisson-Schrödinger solver and the resolution of the Master equation [3,4], the thermoelectric properties of a Si-quantum dot-based single-electron transistor operating in sequential tunneling regime are investigated in terms of thermoelectric figure of merit ZT , efficiency and power (cf. Fig 1 and Fig 2.). By taking into account the phonon-induced collisional broadening of energy levels in the quantum dot, **both heat and electrical currents are computed in a voltage and temperature ranges beyond the linear response** [5].

Skills learned

The student will acquire a broad range of skills: in solid state physics (band structure, electron quantum transport, electron-phonon interaction), technology devices, and scientific programming (Fortran and / or C / C++ , Matlab).

Besides, the results that would be obtained during this internship could be easily published in scientific journals. This work could be a relevant preliminary step for a Phd thesis in our group.

Candidate's Profile

Candidates must have a MSc in Physics, Electronics, Materials Science or related disciplines. We are seeking creative and highly motivated individuals well trained and skilled in scientific research, and available to collaborate in an interdisciplinary team. Programming experience is also desirable, but not mandatory.

Please join a CV, a list of courses that you have followed and results of exams in the framework of your master program, and any other information that you judge useful.

References:

- [1] Zhi-Gang Chen, Guang Han, Lei Yang, Lina Cheng, Jin Zou, "Nanostructured thermoelectric materials: Current research and future challenge", In Progress in Natural Science: Materials International, Volume 22, Issue 6, Pages 535-549 (2012) <https://doi.org/10.1016/j.pnsc.2012.11.011>.
- [2] Mahan, G. & Sofo, J. The best thermoelectric. Proc. Natl. Acad. Sci. 93, 7436–7439 (1996). DOI 10.1073/pnas.93.15.7436
- [3] Talbo, V., Galdin-Retailleau, S., Valentin, A. & Dollfus, P. Physical simulation of silicon-nanocrystal-based single-electron transistors. IEEE Transactions on Electron Devices 58, 3286–3293 (2011). DOI 10.1109/TED.2011.2161611
- [4] Vincent Talbo, Jérôme Saint-Martin, Sylvie Retailleau, and Philippe Dollfus, "Non-linear effects and thermoelectric efficiency of quantum dot-based single-electron transistors", Scientific Reports, 7, 14783 (2017). <https://www.nature.com/articles/s41598-017-14009-4>
- [5] G. Benenti, G. Casati, K. Saito, et R. S. Whitney, "Fundamental aspects of steady-state conversion of heat to work at the nanoscale", Physics Reports, vol. 694, p. 1-124 (2017).