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Research Article

Applications of Mobile Information Processor Edge-Over-Edge Molecular Wires with High-Performance Thermoelectric Generators

J. S. Binoj,[1] Shukur Abu Hassan,[2] Reefat Arefin Khan ,[3] and Alamry Ali[4]

[1].*Micromachining Research Centre, Department of Mechanical Engineering, Mohan Babu University+Tirupati, 517102 Andhra Pradesh, India*
[2]*Centre for Advanced Composite Materials, Office of Deputy Vice-Chancellor (Research & Innovation), Universiti Teknologi Malaysia, Johor Bahru, 81310 Johor, Malaysia*
[3]*College of Business Administration, IUBAT-International University of Business Agriculture and Technology, Dhaka, Bangladesh*
[4]*Department of Mechanical Engineering, College of Engineering in Al-Kharj, Prince Sattam bin Abdulaziz University, Al-Kharj 11942, Saudi Arabia*

Correspondence should be addressed to Reefat Arefin Khan; reefat.arefin@iubat.edu

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If high-efficiency organic isotherm models for mobile processors can be found, a variety of energy harvesting devices, such as Peltier coolers composed of flexible and transparent thin-film materials, might be manufactured. The thermoelectric characteristics of three zinc porphyrins (ZnP) were studied. Theoretical analyses of electron transport across a potassium (Zn-Diphenyl porphyrin: Zn-DPP) molecular sandwiched between electrode surface with three distinct connections were investigated. The contribution of this research is to see what happens because once pyridine is added above the surface of the zinc-porphyrin skeleton, the "edge-over-edge" dimer created from stacked formed rings has a high electrical conductance, minimal exciton thermal conductance, and a large thermal diffusivity on the order of 300 V K1. At room temperature, these variables add up to a projected ZT 4 figure of merit, the greatest ZT for a single organic molecule ever seen. The stacked arrangement of the porphyrin rings causes low phonon thermal conductance, which delays phonon transport across the edge-over-edge molecule and increases the Seebeck coefficient, resulting in a higher ZT value.

1. Introduction

Organics have indeed been employed as active elements in digital devices in molecular electronics, which is a good-looking option for next-generation electronic devices. Understanding charge transport across single-molecule crossings is essential for molecular electrical design procedure, management, and development. Many research have provided insight on topics like resonant charge transfer and the influence of molecular conformation inside the chemical junction throughout the last decade [1]. Several experimental studies have been carried out in order to develop and control electronic molecules that can be used as functional units in future nanoelectronic circuit components such as molecular wires [2].

As a result, the performance of dendrimer circuits is determined by the quality of these components. Metal complexes are an example of a component that is widely employed in nanoelectronic applications. Porphyrins and their derivatives, for example, offer a broad collection of optical and electrical characteristics that allow them to play a vital (important) role in a range of domains, including biological processes, catalysis, electronics, photonics, and nonlinear optics. Metalloporphyrin is made up of a planar aromatic system with a hole in the centre that may house various metals such as Co, Zn, Fe, and other metals. In the last decade, porphyrins and metalloporphyrins have been extensively studied experimentally [3–7] and theoretically [8].

In this paper, we present a theoretical comparison of charge transport characteristics through a single-molecule structure of zinc porphyrin sandwiched between gold electrodes in three different connections, Roth, Meta, and para, as shown in Figure 1, as well as an investigation of the effect of adding pyridine above the surface of zinc-porphyrin in these three cases, as shown in Figure 1. In other words, for these three examples, study the transmission properties and empower S in the absence and presence of pyridine. The characteristics that emerge in the transmission curve in the presence of pyridine in all situations Roth, Meta, and para, as well as their influence on the empower S. The slope of $T\ (E)$ at the Fermi energy EF is proportional to empower S, according to the Mott formula (Equation (1)), where KB, e , and T are the Boltzmann constant, electron charge, and temperature, respectively [9–12].

$$S(E_F, T) \approx \frac{\pi^2 K_B^2 T}{3e} \left(\frac{\partial \mathrm{in}(T(E))}{\partial E} \right)_{E=E_F} \qquad (1)$$

2. Results of Experiments

The implementation of the established offloading optimization techniques is determined in this section. Hunting strategies used by bald eagles are studied for their performance and behavior. To get a better outcome, the various approaches were compared. Critical performance parameters are the' required latency and consider a multiuser in an IoT network in a mobile edge computing (MEC) condition. In this portion, IoT devices are strewn around a 1 km radius, with edge servers strewn about as well. The IoT device area is one of the most important components of the 5G cellular network. In this experimental conclusion, many different users can choose from a variety of offloading end points to which they can submit their work. Our suggested method aims to lower total latency by assigning all workloads from various IoT devices to the best edge servers.

To index diverse network sizes in terms of edge servers, the average power paid on every episode time interval task was employed. When compared to previous methodologies such as DQN and DDPG using network data from local to edge computing, a number of users (users 1, 2, and 3) employ algorithms. The BES approach is intended to improve the result because of the average reward.

As can be shown, the task complexity arrival rate of offloading latency via local is comparable for all user sizes. The number of users increased, and the time it took to send data from edge computing to local decreased. Using local edge computing reduces task complexity and task arrival time.

The BES approach, in comparison to the implementation of average power for the assigned task traffic load per Mbps, is based on edge computing and is granted on per recurrence interval tasks all over various network sizes in terms of edge servers, and the BES technique is particularly in comparison to the execution of average output for the

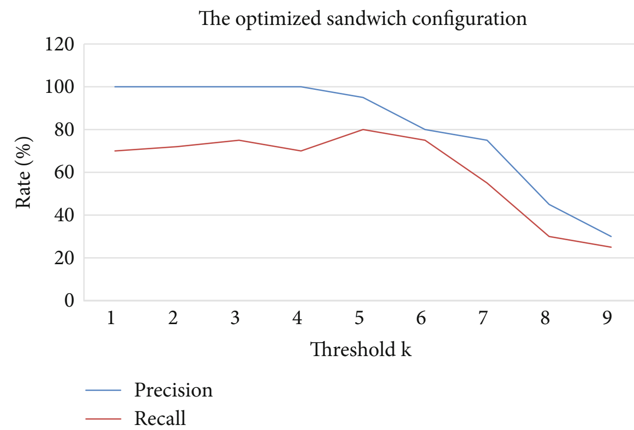

Figure 1: The optimized sandwich configuration of Zn-diphenyl porphyrin.

appointed task arrival rate per Mbps, which is based on the edge of the network and is granted on per recurrence duration tasks across various network sizes in terms of edge servers. The nearer-edge computing network, which handles more subtasks and has more possibilities for avoiding and lowering power consumption by leveraging the edge serve on task, must finally offer data and search here to future local region.

As shown in the figure, the maximum latencies or average buffering delays for distributed offloading on local and BES are measured in milliseconds. For each job's task arrival rate to local on edge computing, the BES approach was used to achieve latency and buffers delay between local and edge computing. This suggests that our technique is more effective than the one before it. This paper's recommended approach technique opens up new possibilities for enhancing latency and dumping efficiency over time. Researchers utilize the performance measures as estimate indicators to see how well the estimating method works. Performance measurements like precision (prec = X/Y) are used to determine the accuracy of ROS selection. Member ROSs that effectively fulfill the user QoS are given a proportion of all ROSs. Rec = X/ACRec = X/ACRec = X/ACRec = X/AC Rec = X/ACRec = X/ACRec = X/ACRec = X/ACRec = X/AC Recall your memories. The percentage of all successfully matching ROSs for which the candidate ROSs successfully match the user account is known as recall (Rec).

The morphologies of isolated silver cyanine molecules were first heated to an optimum configuration using the DFT tool SIESTA. The GGA-PBE implemented double-polarized basis sets.

[24–27]. To compute traditional transport properties, the zinc porphyrin molecule was linked to two gold leads using a thiol group, as shown in Figure 1.

As shown in Table 1, the transmission coefficient T for each relaxed structure represented in Figure 1 was determined using the GOLLUM algorithm [28]. Before evaluating transport characteristics in the presence of pyridine, we first looked at the ideal distance between zinc porphyrins and pyridine. The binding energy EB between zinc porphyrins and pyridine is calculated using the counterpoise technique

Table 1: Number of sensors.

Object	Description	Syntax	Permission
SNumber	Number of sensors in the IoT device	INTEGER	readonly
STable	List of sensors present in the device	SEQUENCE of sEntry	notaccessible
SEntry	Input containing information from a sensor	sEntry	notaccessible
SIndex	Contains sensor information/sensor type	INTEGER	readonly
SDescr	Sensor operation configured status	DisplayString	readonly
SType	Sensor type	INTEGER { List of sensor types}	readonly
SStatusAdmin	Sensor operation configured status	INTEGER { up (1), down (2)}	read&write
SOperator status	Current status of sensor operation	INTEGER { up (1), down (2)}	readonly

Table 2: Communication Comparison.

Attribute	MQTT	SOAP	REST
Allows data exchange	Yes	Yes	Yes
Allows file sharing	No	Yes	Yes
Resource consumption	Low	High	Half
Security measures	Medium (SSL/TLS)	High (WS-security and SSL/TLS)	Medium (SSL/TLS)

as a function of the vertical distance between the nitrogen (in pyridine) and the zinc atom of the porphyrin. As illustrated in Figure 1, we relaxed more from this ideal spacing to get the most energetically favorable arrangement for Roth, Meta, and para connections. Using the same method as before, we compute $T\ (E)$ for each relaxed structure given in the figure using the GOLLUM algorithm [29–32]. We calculated the thermopower S over a wide range of Fermi energies in Table 2 using the equation

$$\mathrm{S} = -1/eTL1/L0 \tag{2}$$

where T is the temperature, e is the electron charge, and Ln is calculated as

$$L_n = \int_{-\infty}^{\infty} (E - E_F)^n T(E) \left(- \frac{\partial f(E, T)}{\partial E} \right) dE \tag{3}$$

where $f(E, T)$ is the Fermi-Dirac probability distribution function which will be noted in Table 2.

3. Conclusions

In summary, we have theoretically examined the transmission characteristics of para, Roth, and Meta zinc porphyrin chemical junctions in the absence and presence of pyridine using the density functional theory DFT simulations. The presence of pyridine above zinc porphyrin has a considerable influence on the transmission coefficients, according to our findings. In the presence of pyridine, those interference characteristics have the ability to affect the value and amplitude of thermopower.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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