Nanocommunication: PHY Advancements in Electromagnetic and Molecular Approaches

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***Abstract*—The field of nanocommunication has recently gained significant attention due to its potential for revolutionizing the way we communicate and process information. This paper covers two main areas of nanocommunication: electromagnetic (EM) and molecular nanocommunication (MNC). EM nanocommunication uses signals in the terahertz (THz) band whereas MNC involves the exchange of information using molecules as carriers. Both approaches have received increasing attention in last decade due to their potential for enabling nanocommunication in challenging environments, such as in-body and on-chip communications. This paper discusses the current state-of-the-art in both paradigms, including the types of modulation recently proposed, the methods for encoding and decoding information, and the challenges. We provide a short survey of the recently proposed works and identify promising directions for future research.**

***Index Terms*—Terahertz band, molecular nanocommunication, diffusion, machine learning, multi-level modulation.**

I. Introduction

In the past few decades, we have witnessed remarkable advancements in communication technologies, leading to a significant transformation in the way we communicate and process information. Nanocommunication [1] is the study of communication at the nanoscale, where devices and networks are designed to operate in the nanometer to micrometer scale. Nanoscale communication has gained significant attention in recent years due to its potential for enabling novel applications in various domains, including healthcare [2], environment [3], and military [4]. One of the most promising applications of nanocommunication is in healthcare. Nanocommunication can enable targeted drug delivery, where drugs are delivered to specific cells or tissues using molecular signals [5]. This can significantly improve the efficacy of drugs and reduce side effects. In addition, nanocommunication can also be used for early disease detection, where molecular signals are used to detect biomarkers associated with various diseases, which can lead to earlier diagnosis and treatment.

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There are two main paradigms of nanocommunication: electromagnetic (EM) [1] and molecular nanocommunication [6]. EM nanocommunication involves the use of EM waves in the Terahertz (THz) band to transmit information at the nanoscale. It is a widely researched topic in the last decade and is typically performed using ultra-short Gaussian pulses [7]. EM nanocommunication is well-suited for ultra high speed communication over short distances providing a data rate in the order of Tbps. Leveraging the unique properties of nanomaterials, such as Graphene, plasmonic communication is possible at nanoscale, a technique that uses surface plasmon polaritons (SPPs) to transmit information [8].

The second most researched area of nanocommunication is molecular nanocommunication, which involves the exchange of information using molecules as carriers [9]. It has emerged from the observation that many biological systems that uses chemical signals to communicate with each other. In molecular communication, information is encoded in the concentration, type, or timing of the molecules released by the nanotransmitter, and is decoded by the nanoreceiver by measuring the concentration, type, or timing of the molecules [10]. Molecular communication offers several advantages over EM communication, such as the ability to operate in challenging environments, such as in biological systems, where EM waves are attenuated or absorbed. Molecular communication also offers a high degree of security and privacy, as the molecules can be confined to a specific area, and their diffusion can be controlled. A comparison of both methods are presented in Table I. In this paper, we mainly focus on the physical layer (PHY) aspects of the nanocommunication.

The rest of this paper is organized as follows. Section II describes the EM nanocommunication mechanism with state-of-the-art modulation schemes and detection mechanisms including the THz channel characteristics. Section III describes the molecular nanocommunication with machine learning method. We provide the molecular channel environment as well as the information encoding and decoding mechanisms. Section IV provides the simulation results of both paradigms. Finally, Section V provides the conclusion with challenges and future works.

II. EM Nanocommunication

A. EM Nanocommunication Channel

Nanocommunication leads to nanonetworks, where multiple nanomachines communicate among each other to perform a common goal. The frequency bands for nanonetworks is proposed to be in the range of 0.1-10 THz [1]. THz band can operate better than any other frequencies for the nanonetworks. This is because when the transmitted noise PSD is considered flat over the entire band, THz band shows negligible losses for fews tens of mm distance, reaching the capacity of $10^2 - 10^3$ Tbps [11]. However, as the distance is increased, the THz channel shows the effect of molecular absorption effects, which creates peaks of attenuation whose frequency depend on the molecular composition of the medium. In addition, there may be losses due to particle scattering and the effects of rain, fog, and clouds.Thus, the propagation model in THz band can be given as

$$A(f, d) = A_{spr}(f, d)A_{mol}(f, d), \quad (1)$$

where $A_{spr}(f, d)$ is the spreading loss and $A_{mol}(f, d)$ is the molecular absorption loss. As a result, the power of THz signal is attenuated, while the noise is amplified. In addition, there is temporal broadening which is incurred by the frequency-selectivity of the channel. Overall, propagation losses have shown an almost linear increase with frequency of operation and transmission distance, while an increase in concentration of molecules has shown to have a major effect on the propagation.

For the transmission of information bits, the most basic signal employed in the nanonetwork is ultra-short Gaussian pulses. In particular, the Gaussian pulses are of 100 fs width, however, the performance could be optimally tuned by varying the shape of the pulse and pulse duration. Fundamentally, the signal can be given as [11]

$$p(t) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(t-t_0)^2}{2\sigma^2}}, \quad (2)$$

where t is the time, t_0 is the time at the center of the pulse, and σ is the standard deviation of the pulse.

B. Pulse-based Modulations

Modulation is the primary element for reliable wireless EM nanocommunication. Considering unique channel properties in the THz band, classic modulation schemes need to be revisited while new ideas to be developed. For instance, as nanocommunication is primarily a short-range communication, ultra-low transmission power and low-complexity implementations are required. Moreover, for very short distances, molecular absorption loss is almost negligible, providing an opportunity to use the THz band as a almost 10 THz wide window. One of the first works to propose modulation was Time-Spread On Off Keying (TS-OOK) [7]. Time spread refers to the phenomenon where the transmitted signal spreads in time to increase the separation between pulses and avoid temporal broadening effects. In TS-OOK, the presence or absence of the pulse represents binary values of 1 or 0, respectively. The pulses are around 100-fs long leading to bandwidths in the THz range. The authors confirms the achievable capacity is in the order of Tbps. In addition, owing to the long time between pulses, TS-OOK can be used for multiple access.

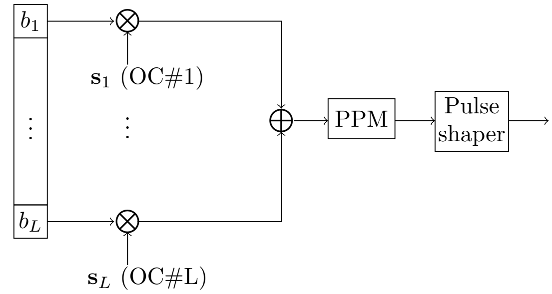

Fig. 1. Transmitter block diagram of the proposed MC-PPM scheme.

In this regard, another scheme proposed is Time Hopping Pulse Position Modulation (TH-PPM) [12]. It combines the advantages of Time Hopping (TH) and Pulse Position Modulation (PPM) to achieve high data rates, good spectral efficiency, and low power consumption. After pulse position modulating the signal, they are further modulated by TH sequence. One of the big advantage of TH-PPM is that it can achieve very high data rates, up to several Tbps, because each pulse can carry multiple bits of data. Another advantage is that it has good spectral efficiency, meaning that it can transmit a large amount of data over a same frequency band. However, the disadvantage is that TH-PPM is sensitive to timing errors, which can cause inter-symbol interference (ISI) and degrade the quality of the received signal. Therefore, accurate synchronization between the transmitter and the receiver is critical to minimize timing errors.

More recently, multi-level pulse position modulation (ML-PPM) has been proposed as another modulation scheme for nanocommunication [13]. In ML-PPM, orthogonal codes have been used to transmit different symbols in different intervals. As shown in Fig. 1, the transmit bits are first multiplied by the respective orthogonal codes and then aggregated to make the multi-levels. These multi-levels are then converted to the pulse positions. The main advantage of ML-PPM is transmission more number of bits per symbol, thereby increasing the data rate of the system. This is because in ML-PPM, by using the orthogonal codes, the multi-levels are converted to pulse positions. These pulse positions represent the specific data.

TABLE I
A COMPARISON OF EM AND MOLECULAR NANOCOMMUNICATION

Attribute	**EM Nanocommunication**	**Molecular Nanoommunication**
Communication signal	Uses EM pulses, typically in the THz band	Relies on the exchange of molecules (chemical signals)
Propagation mechanism	free-space path loss, molecular absorption	Diffusion, molecular absortion
Range	Up to $1\,\mathrm{m}$	Up to $1\,\mathrm{mm}$
Data rate	Up to $1\,\mathrm{Tbps}$	Up to $100\,\mathrm{Mbps}$
Modulation schemes	Ultra-short Gaussian pulse-based including TS-OOK and TH-PPM	Concentration, type, and timing-based encoding
Energy consumption	Energy harvesting	Energy harvesting, generation thorugh chemical processes
Applications	Software-defined metamaterials, wireless robotic materials, in-body communication, on-chip communication	Biological and medical applications, drug delivery, nanomedicine
Experimental challenges	Developing and implementing THz communication devices	Controlling and manipulating molecular signals
Security	Similar to traditional wireless communication	Offers inherent security due to the specificity of molecular signals
Simulation tools	Matlab, NanoSim, COMSOL Multiphysics, BitSimulator, TeraSim	Cellarator, CellDesigner, E-Cell, Discovery Studio, PathVisio, PyMOL

Moreover, in conventional PPM, we can't obtain the spreading gain. However, ML-PPM also has some disadvantages. One major disadvantage is the relatively increased complexity of decoding at the receiver. Since each symbol represents multiple bits of information, the receiver must be able to accurately decode the multi-levels in order to retrieve the transmitted data. On the other hand, ML-PPM is more resilient to noise and interference, as errors in a single bit will not necessarily corrupt the entire symbol.

The signal transmitted by a nanodevice using ML-PPM technique, which conveys information only through time-shifts, can be expressed as follows:

$$s(t) = \sum_{m=0}^{\infty} \sum_{n=0}^{N_p-1} p\left(t - mT_s - nT_f - \mathcal{P}_{d_m(n)}\delta\right). \quad (3)$$

The signal waveform $p(t)$ is the first derivative of a Gaussian pulse, having duration T_p. The term T_f represents the frame duration and n denotes the frame index. The modulation time-shift parameter is given by δ whereas $\mathcal{P}_{d_m(n)}$ controls the pulse-position modulation through the use of $d_m(n)$. The symbol duration T_s is the product of N_p and T_f, where N_p is the number of frames per symbol. Refer to Fig. 2 for a visual representation of the tranmitted symbol.

C. Non-Coherent Detection

To maintain the simplicity of the nanocommunication, we used the non-coherent energy detection receiver. The received signal at the nanoreceiver, denoted as $r(t)$, is modeled as

$$r(t) = s(t) * h_{em}(t) + n(t), \quad (4)$$

where $h_{em}(t)$ is the THz channel impulse response, and $n(t)$ includes noise. We use hard decision decoding at the nanoreceiver, which assumes exact synchronization with the nanotransmitter. The received signal is first integrated over each frame and then sampled. The resulting decision variable $y_{n,l}$ for each frame is obtained as follows

$$y_{n,l} = \int_{nT_f+l\delta+\tau}^{nT_f+(l+1)\delta+\tau} r^2(t)dt, \quad l = 0, 1, ..., L, \quad (5)$$

where $n = 0, ..., N_p - 1$ and $r^2(\cdot)$ is received squared signal. Based on the Maximum-Likelihood decision rule, the multi-level PPM signal and the multi-level signal can be then be demodulated.

III. MOLECULAR NANOCOMMUNICATION

Molecular nanocommunication is another emerging field of research in nanocommunication that seeks to develop communication systems that rely on molecules to transmit information between devices [6]. Devloped just more than a decade ago, although molecular nanocommunication is still in its infancy, several application specific end-to-end molecular nanocommunication models are presented in literature [14]. Moreover, several kinds of encoding schemes are presented of which the most famous is concentration-based encoding

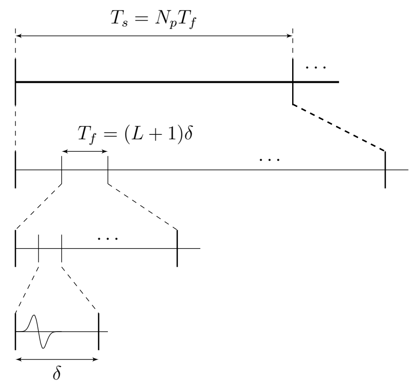

Fig. 2. Signaling structure of the proposed MC-PPM scheme.

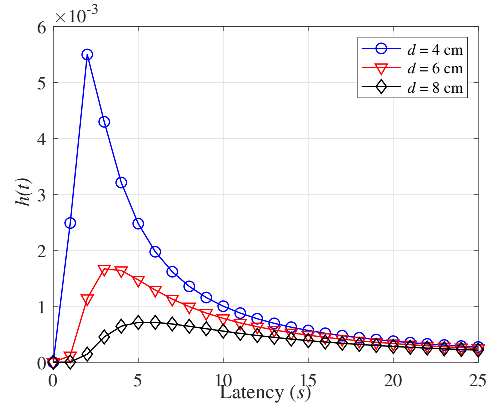

Fig. 3. Impulse response of a pure random walk molecular communication channel with $D = 0.43\ \mathrm{cm}^2/\mathrm{s}$ [17].

[15]. It is a simple encoding scheme that uses different concentrations of molecules to represent different symbols. In this scheme, the transmitter releases molecules into the environment at different concentrations, and the receiver detects the concentration of the molecules to determine the transmitted symbol. The advantage of this scheme is its simplicity, but it is susceptible to interference and noise. In this paper, we present concentration-position shift keying, which is a combination of concentration-based encoding and PPM. For the decoding, we use machine-learning based receiver [16]. As molecular communication is more prone to noise, propagation delay, and ISI in the channel, a machine-learning receiver seems to be a better choice than the conventional receiver.

A. Molecular Nanocommunication Channel

In this study, a most fundamental molecular channel based on pure random walk [10] is considered. A random walk is a mathematical model that describes the movement of a particle or molecule in a medium by random motion. In a pure random walk, the direction and magnitude of the particle's movement are determined solely by chance, with no preference for any particular direction. In other words, there is no directional drift of information molecules and no chemical reaction of information molecules during propagation. Assuming that the distance between the sender and the receiver nanomachine is d, in a medium with diffusion coefficient D, the concentration of the molecules at the nanoreceiver is given as [17]

$$h(t) = \frac{1}{\sqrt{4\pi D t^3}} \exp\left(-\frac{d^2}{4Dt}\right). \tag{6}$$

The above equation can be interpreted at the impulse response of the diffusion channel in 1D environment with an absorbing receiver.

Assume that the sender encodes information onto an information molecule and releases it at time $t = 0$. Fig. 3 indicates the probability of obtaining the molecule at the receiver after the random walk. In particular, Fig. 3 shows the impulse response and the delay for various distance between the sender and receiver. We can observe that the latency is greatly affected by the distance. The average latency for a receiver at any location is infinity, which means that a receiver is expected to wait for infinitely long time to receiver the information molecules. We can observe that the jitter is also infinity.

B. Information Encoding

For the encoding of information, we propose concentration position-shift keying (CPSK), in which information is encoded as the position of the molecular concentration. This can be visualized as analogous to PPM used in EM nanocommunication. In our proposed system, we use M-CPSK modulation to transmit data bits. For instance, in case of 4-CPSK, we modulate '01' in position 2 and '10' in position 3 of the symbol slot. The molecular concentration of the transmitted signal is transmitted at different times. The transmitted molecules pass through the molecular channel and are received by the nanoreceiver through the ligand-receptor binding process (LRBP). Then, the received molecular concentration for each of the M candidate positions is computed by the LRBP process. However, due to channel delay and other factors, some molecules may not be bound by the ligand and remain in the channel or get received in the next time slot or symbol interval resulting in ISI. Mathematically, the signal $Q(t)$ transmitted by sender using the M-ary CPSK modulation can be represented as [17]

$$Q(t) = \begin{cases} Q_s, & \text{if } (m-1)T_s \le t \le mT_s \\ 0, & \text{otherwise} \end{cases}, \tag{7}$$

where $m(\in \{1, 2, ..., M\})$ represents the position of the pulse, Q_s stands for molecular concentration per symbol, and T_s is the time at which molecules are released. We can reformulate above equation as [17]

$$Q(t) = Q_s \sum_{j=-\infty}^{\infty} p\left(t - jT_{tx} - (m-1)T_s\right), \tag{8}$$

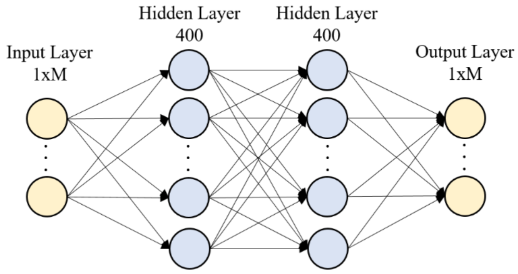

Fig. 4. Machine learning system model for 2-ary and 4-ary CPSK [17].

where $p(t)$ is a normalized concentration shaping function.

C. Information Decoding

When the ligand molecules released by the sender reach the receiver, they collide with the receptor proteins on the surface of the receiver nanomachine. The binding of the ligand to the receptor triggers a biochemical reaction that produces a chemical signal. The strength of the LRBP signal depends on the number of ligand molecules that bind to the receptor, which in turn depends on the concentration of ligand molecules [18], [19]. Mathematically, after passing through the molecular channel, the signal arriving at the receiver can simply be given as [17]

$$U(t) = Q(t) * h(t). \tag{9}$$

1) Machine learning-based receiver: In traditional molecular communication systems, the receiver nanomachine detects the concentration of molecules using its receptors and decodes the information using a pre-defined threshold. However, this approach may not be optimal in free diffusion scenario, where the channel latency and ISI are the main degrading factors. A machine learning-based receiver uses machine learning algorithms to improve the performance of the receiver by learning from the received data. The receiver uses a neural network to estimate the transmitted symbol based on the received molecular concentration values. The neural network is trained using a dataset of known input-output pairs. Once the network is trained, it can estimate the transmitted symbol even in the presence of noise and interference. The machine learning-based approach has several advantages. First, it can adapt to changes in the channel conditions and optimize its performance accordingly. Second, it can learn from experience and improve its performance over time. The model used in the current study are shown in Fig. 4.

During the training process, the input and output values are provided to the machine learning algorithm. The probability values obtained through LRBP are used as input while the transmitted pulse positions are set as the output data. The proposed algorithm is considered as a multilevel classification problem where M positions are classified by learning through the corresponding input-output data pairs. The model in Fig. 4 consists of input, hidden, and output layers. The number of neurons in the hidden layers determines the depth of the neural network and impacts the performance. However, having too many neurons may lead to difficulties in making decisions.

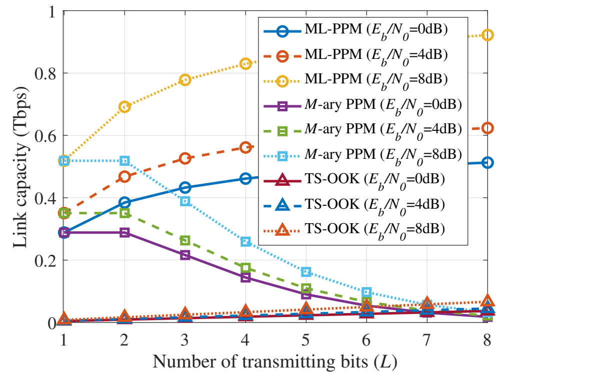

Fig. 5. Performance comparison with other schemes considering d =0.5 mm and Np = 8. The value for TS-OOK is taken to be 1000.

IV. Simulation Results

A. EM Nanocommunication

In this section, we present numerical results for evaluating the performance of the proposed scheme in terms of link capacity. To calculate the link capacity C_L of our scheme, we set the pulse duration as $T_p = \delta$, frame duration as $T_f = (L+1)\delta$, and symbol duration as $T_s = N_p T_f$. Then, the link capacity C_L is calculated as $C_L = (1 - P_b) \cdot C_{L,max}$ where P_b is the bit error rate and $C_{L,max}$ is the maximum link capacity given by

$$C_{L,max} = \frac{L}{T_s} = \frac{L}{N_p(L+1)\delta}. \tag{10}$$

In order to conduct simulations, we generated a first derivative of a Gaussian pulse with a total duration of $2\,\mathrm{ps}$ and a center frequency of $1.6\,\mathrm{THz}$. The energy of the transmitted pulse is dependent on the bit energy E_b, which we maintained at 1 aJ. If all of the bit energy is assigned to a pulse, the nanomachine can transmit one pulse with energy E_b. Walsh-Hadamard codes were used to create the multi-level signal for the orthogonal codes. The THz channel with a water vapor concentration of 10% was used at different communication distances. We used the average concentration of atmospheric gases in a dry atmosphere for other gases, as reported in [11]. In addition, the experiment considered one pulse per frame. We performed 10,000 Monte-Carlo runs for the simulation.

In Fig. 5, we present a comparison of our proposed ML-PPM scheme with other existing nanocommunication modulation techniques, namely TS-OOK [7] and M-ary PPM [12], where M represents the modulation order and $L = \log_2(M)$. To ensure a fair comparison, we use a repetition code of length

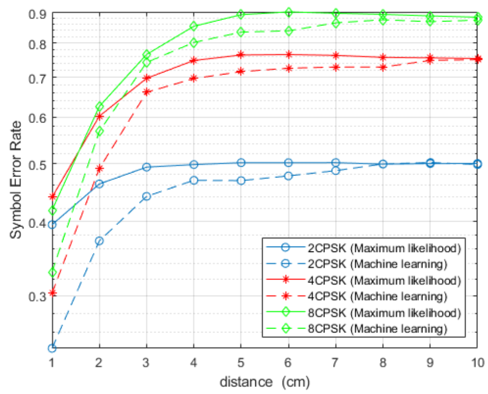

Fig. 6. Symbol error rate performance according to sender-receiver distance and modulation order M [17].

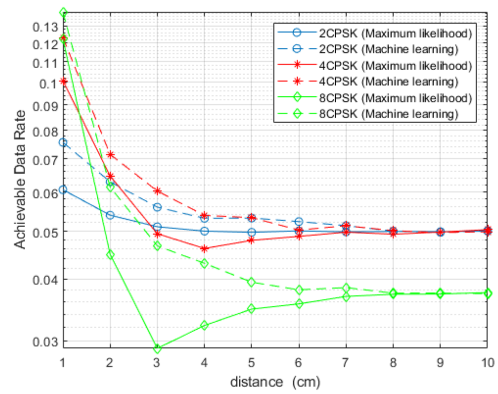

Fig. 7. Achievable data rate performance according to sender-receiver distance and modulation order M [17].

eight and hard decision decoding, with the same processing gain and detection rule for both ML-PPM and M-ary PPM schemes. For TS-OOK, a much longer duration between symbols is used, i.e., $\beta = 1000$ [7]. As depicted in the figure, when transmitting a single bit, the data rate of both ML-PPM and M-ary PPM is the same. However, as the number of transmitting bits increases, the link capacity of ML-PPM exceeds that of PPM. In contrast, the link capacity of M-ary PPM decreases as the number of transmitting bits increases. This is the primary advantage of our proposed ML-PPM scheme over other modulation techniques. Additionally, TS-OOK exhibits much lower data rates.

B. Molecular Nanocommunication

Fig. 6 depicts the effect of modulation order when the total transmission time is fixed at 10 s. For instance, with 8-CPSK, the influence of channel bias (the influence of the channel spreading backward) is seen more compared to 4-CPSK and 2-CPSK. In fact, the SER decreases from d = 3 cm. Therefore, we can say that if we have a longer transmission time, we can reduce the ISI and get better SER performance. This is because the longer symbol duration possesses the channel delay [17].

Fig. 7 illustrates the achievable data rate performance of the proposed CPSK modulation. As expected, the amount of data transfer per unit of time decreases as the distance increases. This is because the number of molecules reaching the receiver decreases significantly with a large distance. However, interestingly, we observe that in the case of the MLE receiver, the ADR does not decrease continually but tends to decrease and then increase. The reason for this kind of behavior is again the bias of the channel quantum response. Note that as the distance increases, the CQR tends to become flat. We can say that 4-CPSK is the sub-optimal case if we take into account the error performance as well as the achievable data rate performance of the proposed scheme. The reason for this is the MC channel's ISI property. Therefore, we can conclude that in the case of MC, even if we increase the modulation order, the data rate reduces because of more errors inhibited in the transmission and propagation.

V. Conclusion, Challenges, and Future Works

This paper discusses the recent work in the EM and molecular nanocommunication. We first discussed the EM nanocommunication and presented the various modulation schemes that can enable EM nanocommunication in the THz band. Then, we discussed the molecular nanocommunication and presented concentration encoded molecular communication with the machine learning nanoreceiver. We have compared our proposed schemes with the convetional schemes in both the paradigms and show a better performance. Still there are several PHY challenges such as nanoantenna design and optimization, network architectures, and more sophisticated channel modeling. As a future work, we are working on finding the solutions to other PHY challenges such as channel coding and estimation.

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