

# **Sensitivity‑Enhanced Surface Plasmon Resonance Sensor**  with Bimetal/ Tungsten Disulfide (WS<sub>2</sub>)/MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) Hybrid **Structure**

**Maryam Ghodrati1 · Ali Mir<sup>1</sup> · Ali Farmani1**

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## **Abstract**

This work aims at improving the sensitivity of a surface plasmon resonance (SPR) sensor with the BK7 prism, silver/gold (Ag/Au) bimetallic films, 2D materials tungsten disulfide (WS<sub>2</sub>), and MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) under angular interrogation technique. The proposed SPR sensor is a free space structure using the Kretschmann confguration to stimulate surface plasmons (SPs). The fnite-diference time-domain (FDTD) method is used to analyze the optical behavior of the proposed SPR sensor. The thickness of the bimetallic layers and the number of layers of 2D materials are optimized to obtain maximum sensitivity for various sensing medium refractive indices ranging from 1.33 to 1.335 RIU. The maximum sensitivity of 348 deg/RIU is obtained with a thickness of 33 nm Ag, a thickness of 15 nm Au and with monolayer  $WS_2$ , and four layers of  $Ti_3C_2T_x$ MXene at 633 nm. This excellent performance of the proposed structure makes it suitable for detecting biomolecules and other analytes.

**Keywords** 2D material · Sensitivity · Surface plasmon resonance ·  $Ti_3C_2T_x$  MXene · Sensor

# **Introduction**

The surface plasmon resonance phenomenon is the resonant coupling of electromagnetic waves to the charge density oscillations at the interface of dielectrics and metals  $[1-3]$  $[1-3]$  $[1-3]$ . Due to the mismatch of optical momentum between the SPR mode and light in free space, the optical excitations in the SPR occur with the attenuated total refection (ATR) method, which was proposed by Kretschmann [[2\]](#page-10-2) and Otto [[3\]](#page-10-1). There is only a TM-polarized electric feld for surface plasmon waves (SPWs). These waves are exponentially decayed at the interface between the dielectric and the metal [\[1](#page-10-0), [3](#page-10-1)[–6](#page-10-3)]. SPR sensors have potential advantages such as real-time and label-free detections, quick response, high sensitivity, cost-efectiveness, high-resolution detection, etc., which has led to their diverse applications [[7–](#page-10-4)[9](#page-10-5)]. Various applications of SPR sensors include environment monitoring, medical diagnostics such as detection of human blood

 $\boxtimes$  Ali Mir mir.a@lu.ac.ir group, DNA, glucose, virus, living cell analysis, and gas sensing [[10–](#page-10-6)[13\]](#page-10-7). In general, noble metals such as gold (Au), silver (Ag), aluminum (Al), and copper (Cu) are widely used plasmonic materials for SPR sensors [[5,](#page-10-8) [6,](#page-10-3) [14–](#page-10-9)[16](#page-10-10)]. Gold and silver are mostly used in SPR sensors because of their excellent chemical stability, better biological affinity, higher sensitivity, and a great fgure of merit in comparison to other metals [\[5,](#page-10-8) [6,](#page-10-3) [17–](#page-10-11)[19\]](#page-10-12). The SPR sensor based on Au shows a broader full width at half maximum (FWHM) that reduces the accuracy of analyte detection while the SPR sensor based on Ag displays higher detection accuracy and lower sensitivity in comparison to Au metal. A bimetallic flm of Ag-Au combines the advantages of both of them, representing its superior candidature for SPR sensors [\[20–](#page-10-13)[22\]](#page-10-14). The 2D materials have desirable physical and structural properties and are well-suited for applications in sensing and biosensing. This is due to great surface adsorption, direct bandgap, and unique optical, chemical, thermal, magnetic, and electrical properties [[23](#page-10-15)[–25](#page-10-16)]. Transition-metal carbides and nitrides, known as MXenes, are 2D materials by the general formula  $M_{n+1}X_nT_{x}$ , where *M* represents an early transition metal, *X* is carbon and/or nitrogen, and  $T_x$  is the surface termination groups ((–O), (–F), and (–OH)) [[7,](#page-10-4) [8,](#page-10-17) [26–](#page-11-0)[28](#page-11-1)]. The *n* index indicates a variable number between 1 and 3. Among

<sup>1</sup> Faculty of Engineering, Lorestan University, Khoram-Abad, Iran

the types of MXene,  $Ti_3C_2T_X$  MXene has shown potential in numerous felds, and due to its unique optical and electrical properties improves sensor performance and quality [\[8,](#page-10-17) [29](#page-11-2)–[31\]](#page-11-3). Transition metal dichalcogenides (TMDs) are a class of 2D materials with the formula  $MX_2$ , where M stands for metal (Molybdenum or Tungsten) and *X* refers to chalcogenide (sulfur, selenium, or tellurium) like  $MoS<sub>2</sub>$ ,  $MoSe<sub>2</sub>, WS<sub>2</sub>, and WS<sub>e<sub>2</sub></sub> offers tunable optical and electronic$ properties [[30–](#page-11-4)[32\]](#page-11-5). In recent years, the various structures of SPR sensors have been studied to improve the performance parameters of sensors, especially sensitivity. Vibisha et al. investigated the use of the TMDCs material over a Cu-Ni bimetallic layer to achieve the higher sensitivity with optimized Cu and Ni layer [[5](#page-10-8)]. Zhao et al. reported the sensor structure using seven layers of  $WS_2$  over Al metal and BK7 prism; the proposed sensor obtained a sensitivity of 315.5 deg/RIU [\[29](#page-11-2)]. Kumar et al. introduced the SPR sensor with Ag-Si-MXene and Ag-Si-BP-MXene to achieve high sensitivity of 231 deg/RIU and 264 deg/RIU, respectively [[30,](#page-11-4) [31](#page-11-3)]. Yue et al. [\[32\]](#page-11-5) proposed a SPR sensor consists of Ag-Au bimetallic structure with BlueP/TMDCs and graphene; the results showed that the sensitivity could be signifcantly increased. Shushama et al. presented an SPR sensor structure consisting of a hybrid structure with a silicon layer, a monolayer of  $MoS<sub>2</sub>$ , and graphene on a BK7 prism; the offered structure improved sensitivity to around 210 deg/ RIU [[33\]](#page-11-6). The Kretschmann confguration is generally documented as one of the most basic SPR confgurations for biosensors, and SPR with a single prism is a frequently utilized technique in sensor application. As mentioned earlier, 2D nanomaterials and their heterostructures like MXenes have extraordinary properties such as high surface‐to‐volume ratio, excellent electric conductivity, and high absorption; also, their surface can be functionalized with various analytes or nanobiomolecules. All these factors make them a suitable platforms for sensor and biosensor development. On the other hand, due to the rising steadily of human disease, we need easy-to-use and detectable sensing systems. Therefore, the development of reliable biosensor systems for multi-analytic detection is another need to be considered. In this regard, we presented a SPR sensor based on the BK7 prism, silver/gold (Ag/Au) bimetallic flms, 2D materials tungsten disulfide (WS<sub>2</sub>), and MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) under angular interrogation technique. The proposed sensor is a free space structure using the Kretschmann confguration to stimulate SPs. There are too many papers reported in the literature which uses the 2D materials for the sensitivity enhancement but based on the knowledge of the authors, the heterostructure proposed based on Ag/Au bimetallic and WS<sub>2</sub>-MXene composites here has not been used before. The novelty of the current paper lies in the use of Ag/Au bimetallic and  $WS_2$ -MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) hybrid structure can efectively detect biomolecules at room temperature. In this

paper, the minimum reflection  $(R_{min})$ , sensitivity, figure of merit (FOM), and detection accuracy (DA) of the SPR curve are investigated using the numerical method of FDTD in the visible regime. The results show by optimizing thickness of the bimetallic and the number of layers of 2D materials; the maximum sensitivity was achieved at 633 nm.

## **Materials and Sensor Design**

The schematic of the proposed SPR sensor based on the Kretschmann structure is illustrated in Fig. [1](#page-2-0)a. The structure consists of six layers, including BK7 prism, Ag/Au bimetallic films, tungsten disulfide (WS<sub>2</sub>), MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>), and sensing medium (SM).

The fnite-diference time-domain (FDTD) technique is used to evaluate electromagnetic feld analysis for the proposed sensor, which is a powerful method to solve Maxwell's equations in a nanoflm layer by using the YEEalgorithms [[17,](#page-10-11) [20](#page-10-13), [25](#page-10-16)]. In fact, a two-dimensional FDTD simulation is used for this analysis. The XY view of the FDTD simulation schematic for the proposed SPR biosensor is depicted in Fig. [1](#page-2-0)b. The parameter sweep is used for angular interrogation over a wide range of source angels (40 to 85°), in order to obtain the source angle capable to excite the SPR mode. The optical parameter was set as a planewave source (Bloch/periodic type) at an optical wavelength of 633 nm. The perfectly matched layer (PML) boundary condition was used in such a way that waves enter into the layers with generating minimum refections. Also, for excitation of the SPW, the incident light is a transverse magnetic (TM) polarized. In proposed structure, we use BK7 prism with  $n_{BK7}$ =1.5151 at  $\lambda$ =633 nm as the coupling prism for exciting SPR. The refractive index (RI) of BK7 can be calculated from Eq.  $(1)$  $(1)$   $[4, 29, 31]$  $[4, 29, 31]$  $[4, 29, 31]$  $[4, 29, 31]$  $[4, 29, 31]$  $[4, 29, 31]$ :

<span id="page-1-0"></span>
$$
n_{BK_7}(\lambda) = \sqrt{\frac{1.03961212\lambda^2}{\lambda^2 - 0.00600069867} + \frac{0.231792344\lambda^2}{\lambda^2 - 0.0200179144} \over + \frac{1.01046945\lambda^2}{\lambda^2 - 103.560653} + 1}
$$
(1)

In Eq.  $(1)$  $(1)$ ,  $\lambda$  represents the wavelength of incident light in µm scale. According to the Drude–Lorentz model, the refractive indexes of the metals are determined by [[29–](#page-11-2)[32\]](#page-11-5) :

$$
n_m(\lambda) = \sqrt{\left(\epsilon'_m + i\epsilon''_m\right)} = \sqrt{\left[1 - \frac{\lambda^2 \lambda_C}{\lambda_P^2 \left(\lambda_C + i\lambda\right)}\right]}
$$
(2)

where  $\lambda_p$  and  $\lambda_c$  represent the plasma and collision wavelength. The values of  $\lambda_p$  and  $\lambda_c$  for Ag are equal to  $1.4541 \times 10^{-7}$  m and  $17.614 \times 10^{-6}$  m, respectively [\[29](#page-11-2)[–32](#page-11-5)], and the thickness of the Ag layer is 33 nm. To reduce the oxidation of the Ag layer, the Au flm is deposited on the Ag layer. Furthermore, the use of a bimetallic structure

<span id="page-2-0"></span>**Fig. 1 a** Schematic diagram of the proposed SPR sensor **b** XY view of the FDTD simulation schematic for the proposed SPR biosensor



enhances sensitivity in the SPR sensor highly. The values of  $\lambda_p$  and  $\lambda_c$  for Au are equal to 1.6826×10<sup>-7</sup> m and  $8.9342 \times 10^{-6}$  m, respectively [\[29–](#page-11-2)[32](#page-11-5)], and the thickness of the Au layer is 15 nm. We have chosen Ag/Au bimetallic flms instead of single plasmonic metal. To stabilize the device, monolayer  $WS_2$  was placed on the metal so that metal can free from the chemical reaction and a huge amount of light energy can be absorbed. The complex RI of tungsten disulfide (WS<sub>2</sub>) is  $n_{WSS} = 4.89 + 0.314i$ , and its thickness is equal to  $d_{\text{WS2}} = L \times 0.8$  nm, where *L* is the number of  $WS_2$  layers, and 0.8 is the thickness of a monolayer  $[29, 1]$  $[29, 1]$  $[29, 1]$ [32](#page-11-5)]. Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene is deposited over WS<sub>2</sub> as a biorecognition element (BRE) layer for analytes due to its hydrophilic nature and large surface area. The complex RI of  $Ti_3C_2T_x$ MXene is  $n_{Mxene} = 2.38 + 1.33i$ , and its thickness is equal to

 $d_{MXene} = L \times 0.993$  nm, where *L* is the number of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene layers and 0.993 is the thickness of a monolayer [[4,](#page-10-18) [7](#page-10-4)]. Finally, the last layer is the sensing medium and the RI of this medium is given as  $n_s = 1.33 + \Delta n_s$ , where  $\Delta n_s$  is the change of RI in sensing medium due to the occurrence of a biological action. We have considered the sensing medium as an aqueous solution with a refractive index of 1.33 RIU and selected the refractive index changes with steps of 0.005 RIU. The adsorption of the molecule on the sensor surface changes the concentration of the aqueous solution, which in turn changes the RI of the sensing medium. In other words, this varies from 1.33 to 1.35 RIU when analyte is adsorbed at the MXene surface. The large surface area of  $Ti_3C_2T_s$ MXene due to its layered nature provides an increased contact area for the attachment of the molecule.

#### **Performance Parameters of the SPR Sensor**

The performance parameters defned for the proposed SPR sensor are sensitivity, full width at half maximum (FWHM), detection accuracy (DA), and fgure of merit (FOM). The FDTD numerical method is used to obtain all the performance parameters. The sensitivity is defned as the ratio of SPR angle shift ( $\Delta\theta_{SPR}$ ) to the changes in refractive index  $(\Delta n_s)$  in the sensing medium by the following equation [[20,](#page-10-13) [30](#page-11-4), [32](#page-11-5)] :

$$
S = \frac{\Delta \theta_{SPP}}{\Delta n_s} \tag{3}
$$

The unit of sensitivity is expressed as deg/RIU. To better understand the sensing performance of the SPR sensors, another intelligent scale of measurement called FOM dimensioned at RIU−1 is used that is obtained from the ratio of the sensitivity to the FWHM based on Eq.  $(4)$  $(4)$  [\[20](#page-10-13), [30,](#page-11-4) [32\]](#page-11-5):

$$
FOM = \frac{S}{FWHM} \tag{4}
$$

where FWHM is a diference of the resonance angles at 50% refection intensity [[29,](#page-11-2) [32\]](#page-11-5). FWHM also shows the angular width of the refectance curve. Another critical parameter of the SPR sensor is the detection accuracy, dimensioned at deg<sup>-1</sup>, and can be determined by taking the inverse of

<span id="page-3-1"></span>

the FWHM of the SPR curve, using the following equation [[29,](#page-11-2) [30,](#page-11-4) [32\]](#page-11-5) :

$$
DA = \frac{1}{FWHM} \tag{5}
$$

# **Results and Discussion**

First of all, we calculated the absorption spectrum of the conventional sensor structure by the numerical simulation and compared it with analytical results of transfer-matrix method (TMM), and the experimental Johnson-Christy model to prove the accuracy of our model. As shown in Fig. [2,](#page-3-1) there is a good agreement between the FDTD simulation with analytical results, and the experimental Johnson-Christy model, which confrms the validity and accuracy of our model. It is clear that the absorption peaks are close to each other. It should be noted that we have only done theoretical research but it is possible to implement it practically.

<span id="page-3-0"></span>Here, we have considered diferent thicknesses of Ag and Au to determine the optimized thickness of bimetals. According to the literature, the metal layer plays a signifcant role in the generation of surface plasmons so the thickness optimization of Ag/Au metals is essential to balance the photon absorption efficiency as well as energy loss. Also, the use of bimetallic Ag/Au layers and 2D materials such as



<span id="page-4-0"></span>**Fig. 3** Variation in **a** resonance angle shift and minimum refection **b** sensitivity, detection accuracy, and FOM versus the Ag/Au thickness of the proposed SPR sensor



**(b)**

 $WS_2$  and  $Ti_3C_2T_x$  MXene over bimetallic Ag/Au layers in the proposed SPR sensor can contribute to sensitivity enhancement. We considered the thickness of the Ag layer equal to 28, 33, 38, 43, and 48 nm, and the Au layer thickness equal to 0, 5, 10, 15, and 20 nm, respectively. Figure [3](#page-4-0)a and b show resonance angle shift, minimum refection, sensitivity, DA, and FOM in terms of Ag/Au thicknesses for the proposed SPR sensor. From Fig. [3](#page-4-0)a, the variation in resonance angle shift is obtained 0.88, 0.94, 0.985, 1.21, and 1.015 deg and the minimum refection is calculated 0.1019, 0.1272, 0.1471, 0.1402, and 0.1666 a.u. for diferent thickness combinations of Ag and Au.

It is observed that the minimum refection less than 0.15 a.u. with high variation in resonance angle shift is obtained at 35:15 nm thickness of Ag and Au metals, respectively. Furthermore, Fig. [3b](#page-4-0) shows the sensitivity, detection accuracy, and fgure of merit of the proposed SPR sensor for diferent thicknesses of Ag and Au. The values calculated for sensitivities, DAs, and FOMs are 176, 188, 197, 242, and 203 deg/RIU, 0.222, 0.163, 0.143, 0.116, and 0.107 deg<sup>-1</sup>, and 39.19, 30.71, 28.18, 28.07, and 21.89 RIU−1, respectively. It is obvious from Fig. [3](#page-4-0)b that the 35:15 optimized thickness ratio of Ag/Au bimetal gives high sensitivity, while DA becomes low due to the broader SPR curve. We describe the role of each of the layered used in the proposed design via the SPR curve. The SPR characteristic curves for four structures include the following: structure  $1 - BK7$ prism/Ag/SM, structure 2 – BK7 prism/Ag/Au/SM, structure  $3 - BK7$  prism/Ag/Au/WS<sub>2</sub>(1L)/SM, and structure 4 – BK7 prism/Ag/Au/WS<sub>2</sub>(1L)/Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene(1L)/SM which are presented in Fig. [4a](#page-5-0)–d, respectively. The inset graphs within Fig. [4](#page-5-0)a–d show the variation of refection with RI of the sensing medium for 1.33 and 1.335 RIU, on the adsorption of biomolecules on the sensor surface. We calculate resonance angle shift for the sensing layer RI variation of  $(\Delta n_{s}=0.005)$  for four structures.



<span id="page-5-0"></span>**Fig. 4** The SPR curves with respect to the incident angle for **a** structure 1, **b** structure 2, **c** structure 3, and **d** the proposed SPR sensor (structure 4)

<span id="page-6-0"></span>**Table 1** Comparison of performance parameter between the proposed sensor with other structures

<b>Parameters</b>	<b>Structures</b>			
	Structure 1	Structure 2	- Structure 3	Structure 4 (proposed)
$\Delta\theta_{res}$ (deg)	0.61	0.69	0.81	1.21
$S$ (deg/RIU)	122.	138	162	242
$\mathbf{R}_{\min}$ (a.u.)	0.0034	0.0203	0.0312	0.1402
DA(1/deg)	0.334	0.258	0.134	0.116
<b>FWHM</b> (deg)	2.99	3.87	7.46	8.62
FOM $(RIU^{-1})$	40.80	35.65	21.72	28.07

Resonance angle shift obtained from SPR curves shown in Fig. [4](#page-5-0)a–d for structures 1, 2, 3, and 4 is 0.61, 0.69, 0.81, and 1.21 deg, respectively. Sensitivity calculated from above resonance angle shift for mentioned structures is 122, 138, 162, and 242 deg/RIU, respectively. The performance parameters FOM, DA, and FWHM calculated from SPR characteristic curves plotted in Fig. [4](#page-5-0)a–d for diferent SPR sensor confgurations are presented in Table [1](#page-6-0). Based on the results, it can be found that embedding the  $Ti_3C_2T_x$ MXene layer in the proposed SPR sensor contributes to

sensitivity enhancement. This is due to the strong charge transfer between  $Ti_3C_2T_x$  MXene /WS<sub>2</sub> layer and bimetallic Ag/Au layers. The decrease in DA and FOM is due to lossy nature of  $Ti_3C_2T_x$  MXene because of larger value of imaginary part of its refractive index. Figure [5a](#page-6-1)–d show the electric feld intensity for structures 1, 2, 3, and 4. As can be seen, the strength of electric feld intensity is enhanced in the proposed SPR sensor (structure 4) compared to the other structures. The layered nature of  $Ti_3C_2T_x$  MXene creates a strong light-matter interaction. In fact, the use of a 2D material MXene increases the electromagnetic feld within the SPs at the metal–dielectric interface. By increasing the electromagnetic feld intensity, the SPP excitation in the sensing area increases and the sensitivity improves.

Figure [6](#page-7-0) shows the absorption curve variation versus the RI of sensing layer from 1.33 to 1.35 RIU on the adsorption of biomolecules on the sensor surface. As can be seen, by increasing the RI of sensing layer, the plasmon resonance occurs at a larger angle. The performance of the sensor depends on the RI variation of the sensing medium. Changes in the RI lead to a change in the absorption curve. We have considered the SPR angle obtained for diferent RI values of sensing layer from  $n<sub>s</sub> = 1.33$  to 1.35 RIU for the step of 0.005 of the sensing medium.



<span id="page-6-1"></span>**Fig. 5** Electric feld intensity for **a** structure 1, **b** structure 2, **c** structure 3, and **d** the proposed SPR sensor (structure 4)

<span id="page-7-0"></span>**Fig. 6** The absorption curve as a function of the incident angle for diferent RI of sensing layer from 1.33 to 1.35 RIU for the proposed structure



Figure [7](#page-7-1) plots the performance parameters variation with sensing layer RI for the proposed SPR sensor. The sensitivity, minimum refection, DA, and FOM of the proposed structure varies from 242 to 287 deg/RIU, 0.1566 to 0.2854 a.u., 0.116 to 0.112 deg<sup>-1</sup>, 28.07 to 32.43 RIU<sup>-1</sup>, respectively, for the RI variation of sensing layer from 1.33 to 1.35 RIU. Also, to consider the effect of thickness of the  $Ti_3C_2T_x$ MXene layer, we plotted the refection curve with one layer, two layers, three layers, and four layers of  $Ti_3C_2T_x$  MXene as shown in Fig. [8.](#page-8-0) The results show that when the number of the  $Ti_3C_2T_x$  MXene layers increases, minimum reflection and the width of the resonance curve increase. In other

<span id="page-7-1"></span>

variation vs. RI of sensing layer for the proposed SPR sensor



<span id="page-8-0"></span>**Fig. 8** The refection curve of the proposed SPR sensor for diferent layers of  $Ti_3C_2T_x$  MXene

words, as the number of  $Ti_3C_2T_x$  MXene layers increases, the damping associated with the SPs wave increases, thereby increasing the FWHM and  $R_{\text{min}}$ .

Based on Fig. [8](#page-8-0), the proposed SPR sensor for the case of four  $Ti_3C_2T_x$  MXene layers shows maximum sensitivity of 348 deg/RIU. Sensitivity improvement is due to better confnement of charge carriers and shifts the SPR resonance angle. The interaction of the hexagonal structure of  $Ti_3C_2T$ , MXene with the analyte leads to an enhancement of the adsorption of biomolecules, and increases the sensitivity to changes in the RI, so the use of MXene improves the sensitivity of the sensor.

Absorption curves for the proposed SPR sensor are ana-lyzed in Fig. [9a](#page-8-1)–d with different TMDs  $(MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>,$ WSe<sub>2</sub>) layers and keeping  $Ti_3C_2T_x$  MXene fixed at the monolayer. It should be noted the refractive indices of the  $MoS<sub>2</sub>$ , MoSe<sub>2</sub>, and WSe<sub>2</sub> are 5.0947 + 1.2327*i*, 4.6226 + 1.0063*i*, and 4.5502+0.4332i, respectively, and thicknesses are 0.65, 0.70, and 0.70 nm, respectively [\[32](#page-11-5)[–36\]](#page-11-7). Resonance angle shifts obtained from SPR curves for  $MoS_2$ ,  $MoSe_2$ ,  $WS_2$ ,



<span id="page-8-1"></span>**Fig.** 9 Absorption curve of the proposed structure for different TMDs: **a** MoS<sub>2</sub> layer, **b** MoSe<sub>2</sub> layer, **c** WS<sub>2</sub> layer, **d** WSe<sub>2</sub> layer

<span id="page-9-0"></span>**Fig. 10** Sensitivity of the proposed SPR sensor vs. the RI of the sensing layer for diferent TMD layers and varying layers of  $Ti_3C_2T_x$  MXene



and  $WSe<sub>2</sub>$  are 1.16, 0.9, 1.21, and 1.01 deg, respectively. Sensitivities calculated from the above resonance angle shifts for  $MoS_2$ ,  $MoSe_2$ ,  $WS_2$ , and  $WSe_2$  are 232, 180, 242, and 202 deg/RIU, respectively. The highest sensitivity is obtained for  $WS_2$ ; this is due to the wavelength-dependent order of light absorbance of TMDs, which is least for  $WS_2$ than  $WSe_2$ ,  $MoSe_2$ , and  $MoS_2$  TMD layers.

Figure [10](#page-9-0) also shows the sensitivity variation in terms of sensing layer RI for the proposed SPR sensor with diferent TMDs ( $MoS<sub>2</sub>$ , MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>) layers and varying layers of  $Ti_3C_2T_x$  MXene. As can be seen, sensitivity raises with an increase in sensing layer RI for each TMDs layer. Because the light absorption capability of  $WSe_2$ ,  $MoSe_2$ , and  $MoS<sub>2</sub>$  layers is higher than  $WS<sub>2</sub>$ , the maximum sensitivity is obtained with the  $WS_2$  layer. Also, with increasing the number of  $Ti_3C_2T_x$  MXene layers from 1 to 4, the sensitivity increases. The highest sensitivity is achieved for the proposed SPR sensor with four layers of  $Ti_3C_2T_x$  MXene.

Table [2](#page-9-1) illustrates the comparison between the proposed structure with the SPR sensors explored by diferent research groups. The proposed SPR sensor shows the highest sensitivity compared to the other structures at 633 nm. The use of  $WS_2/Ti_3C_2T_x$  MXene hybrid structure in the proposed sensor enhances the adsorption of biomolecules due to stronger Van der Waals forces, so this heterostructure improves the performance of the proposed SPR sensor. It is predicted that a novel bimetallic SPR sensor based on the 2D material  $Ti_3C_2T_x$  MXene layer and WS<sub>2</sub> will be useful for medical diagnosis and biological applications. It is anticipated that the proposed work will be able to detect (bio)chemicals with good sensitivity and speed. Since SPR sensors have the potential to detect various types of biological and biochemical analytes. So, research on 2D materials and their heterostructures in sensing and biosensing application requires more theoretical and practical study and has the potential for further development in the coming years. We hope that the



<span id="page-9-1"></span>**Table 2** Comparison of the sensitivity and FOM of the proposed structure to other existing SPR sensors

proposed work would educate researchers about SPR sensors and inspire them to do further research and development in this feld.

## **Conclusion**

In this work, an SPR sensor utilizing a bimetallic layer of Ag/Au with 2D material  $WS_2$  and  $Ti_3C_2T_x$  MXene based on Kretschmann confguration have studied. The diferent parameters of the sensor like sensitivity, DA, FOM, and FWHM had analyzed by using the FDTD method. The proposed SPR sensor has a maximum sensitivity of 242 deg/ RIU with 35 nm of Ag, 15 nm of Au, a monolayer of 2D material  $WS_2$ , and one layer of  $Ti_3C_2T_x$  MXene. Using four layers of  $Ti_3C_2T_x$  MXene over a WS<sub>2</sub> layer, the highest sensitivity of 348 deg/RIU had achieved. We also investigate the function of the bimetallic layers with different TMDs  $(MoS<sub>2</sub>)$ ,  $MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>$ ) layers and found WS<sub>2</sub> layer has a better sensing performance. We expect that such promising results will lead the proposed structure as a potential candidate for detecting biomolecules and other analytes and can be used for biosensing and chemical sensing applications.

**Author Contribution** MG, AM, AF: software, data curation, investigation, conceptualization, methodology, writing — review and editing. AM, AF: validation, data curation, writing — original draft.

**Data Availability** All data included in this paper are available upon request by contact with the contact corresponding author.

## **Declarations**

**Consent for Publication** All authors of this paper agree to publish our theoretical research.

**Competing Interests** The authors declare no competing interests.

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