Supporting Information


Mid-Infrared Silicon-on-Lithium-Niobate Electro-Optic Modulators Toward Integrated Spectroscopic Sensing Systems

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Note S1 Analysis of external confinement factor and electro-optic interaction

The percentage of optical power or intensity confined in the gain medium (or cladding) was typically considered as the waveguide gain. However, for waveguide with notable index-contrast, it has been pointed out by J. T. Robinson et al. that the additional modal gain should be considered in the optical confinement factor using variational theorem. To differentiate from the former expression, here we introduce it as the “external confinement factor”\(^{[1,2]}\):

\[
\Gamma_{\text{ext}} = \frac{n_{\text{clad}} c \varepsilon_0}{\int \Re \{E \times H^*\} \cdot \hat{e}_z dx dy} = \frac{n_g}{n_{\text{clad}}} \frac{\int \varepsilon|E|^2 dx dy}{\int \varepsilon|E|^2 dx dy} = \frac{n_g}{n_{\text{clad}}} \gamma_{\text{ext}} \quad \text{(Equation S1)}
\]

, where \(n_g\) is the group index, \(n_{\text{clad}}\) is the refractive index of the cladding, \(c\) is the speed of light in vacuum, \(\varepsilon\) is the corresponding permittivity of the region, \(E\) is the spatial electric field and \(\gamma_{\text{ext}}\) is the fraction of electric field energy density in the gain medium. From here, only in case \(n_g \approx n_{\text{clad}}\), the value of \(\gamma_{\text{ext}}\) approaches \(\Gamma_{\text{ext}}\) and the two definitions could be used interchangeably.

The same idea has been widely adopted when calculating the sensitivity of waveguide sensors leveraging light-matter interaction via an evanescent field\(^{[3,4]}\).

Namely, it implies a linear dispersion in the medium matching that of the cladding, which is however unrealistic. Substantially, it originates from the incompatibility of the common approximation for the major components of the electric and magnetic field (for \(y\)-propagating TM mode in this case):

\[
E_x = -\frac{\omega \mu_0}{\beta} H_z \quad \text{(Equation S2)}
\]

, where \(\beta\) is the propagation constant, \(\mu_0\) is the vacuum permeability and \(\omega\) is the angular frequency. In our case, as revealed by the noticeable spatial distribution difference between Figure S1a and b, the linear relationship in Equation S2 does not hold as satisfying different boundary conditions.

**Figure S1.** Major components of fundamental TM mode. a) Electric field distribution and b) magnetic field distribution related to electric fields are plotted on the same color scale. The evident difference between spatial distribution is observed.
Therefore, the external confinement factor can be readily calculated from \textbf{Equation S1} for an arbitrary part of the waveguide. Here, the material of interest was lithium niobate (LN) and the corresponding $\Gamma_{\text{LN}}$ can be particularly written as:

$$\Gamma_{\text{LN}} = \frac{n_g}{n_{\text{LN}}} \cdot \frac{\iint_{\text{LN}} \varepsilon |E_{\text{op}}|^2 \, dx\,dy\,dz}{\iint_{\varepsilon} \varepsilon |E_{\text{op}}|^2 \, dx\,dy\,dz} = \frac{n_g}{n_{\text{LN}}} \gamma_{\text{LN}}$$

(Equation S3)

, with $n_{\text{LN}}$ being the refractive index of LN. Considering the electro-optic modulation in hybrid configuration, the relative change of the effective index change $n_{\text{eff}}$ with respect to the local change of $n_{\text{LN}}$ can be expressed as:

$$\Delta n_{\text{eff}} = \Delta n_{\text{LN}} \cdot \Gamma_{\text{LN}}$$

(Equation S4)

The total phase shift of the guided mode due to the material index change in LN is:

$$\Delta \Phi = \Delta \beta L = \Gamma_{\text{LN}} k_0 \Delta n_{\text{LN}} L$$

(Equation S5)

As indicated in \textbf{Figure 4a} in the main text, it is apparent that the electric field in the LN layer is mainly along the $z$-axis and the effective refractive index of the propagating TM mode is subject mainly to the variation for ordinary index $n_o$. According to the Pockels effect,

$$\Delta n_{\text{LN}} = \frac{1}{2} r_{13} n_{\text{LN}}^3 E_{\text{ext}}^z$$

(Equation S6)

The figure of merit used for MZM i.e. halfwave voltage length product can be expressed as:

$$V_{\pi} L = \frac{\lambda_0 g}{2 n_{\text{LN}}^3 r_{13} \Gamma_{\text{eo}}}$$

(Equation S7)

, where $\Gamma_{\text{eo}}$ is the normalized overlap between the optical field and the microwave field within the LN region. Assuming the lateral electric field is continuous and distributed uniformly,[5] it can be approximated as:

$$\Gamma_{\text{eo}} = \frac{g}{V_A} \cdot \frac{n_g}{n_{\text{LN}}} \frac{\iint_{\text{LN}} \varepsilon |E_{\text{op}}|^2 E_{\text{ext}}^z \, dx\,dy\,dz}{\iint_{\varepsilon} \varepsilon |E_{\text{op}}|^2 \, dx\,dy\,dz} \approx \frac{g E_{\text{ext}}^z}{V_A} \Gamma_{\text{LN}}$$

(Equation S8)

From here, we can intuitively relate $\Gamma_{\text{eo}}$ to $\Gamma_{\text{LN}}$ with a certain ratio. It is worth mentioning that in monolithic LN waveguide, $\Gamma_{\text{eo}}$ depends entirely on the electrical design since all the optical mode is intrinsically confined in LN. However, for hybrid waveguide configurations, it is a pivotal design challenge to leak as much light as possible into the LN film. To this end, we leverage the modal gain of the TM-polarized propagating mode to feature a large $\Gamma_{\text{LN}}$, ultimately improving $\Gamma_{\text{eo}}$ in a costless manner.
Note S2 Simulation of subwavelength waveguide

To ensure the precise extraction of spatial electric field distribution and obtain the external confinement factor, three-dimensional finite-difference-time-domain (3D-FDTD) simulations are performed through commercial software Lumerical. The group indices of the guided mode \( \left( n_g = \frac{c}{v_g} = c \frac{\partial k}{\partial \omega} \right) \) involving periodic subwavelength grating (SWG) are extracted from the corresponding band diagrams obtained. Notably, five 3D power monitors are placed as illustrated in the inset of **Figure S2**, including one in air region beneath Si layer (Monitor 1), one in Si waveguide core (Monitor 2), two in periodically alternative SWGs region (Monitor 3 & 4) and one in LN substrate (Monitor 5). The definite integral of \( |E|^2 \) for each monitor in **Equation S3** is approximated as sums of multiple mesh subdivisions.

**Figure S2.** Schematic illustration of the simulation setting for spatial electric field distribution. The inset shows the cross-section of multiple 3D monitors.
Note S3 Design of waveguide and electrode configuration

**Figure S3.** a) External confinement factor $\Gamma_{LN}$ of TE mode with respect to silicon thickness. Mode profiles for b) 500 nm- and c) 220 nm-thick Si layer.

**Figure S4.** a) Simulated propagation loss and external confinement factor variation with respect to different waveguide widths. b) Simulated loss for various 90° bent waveguides with different radius. c) Simulated coupling efficiency of the grating coupler.

**Figure S5.** The optical field profiles a) without electrodes and b) with electrodes. The optical field is not disturbed by electrodes due to distance optimization.
Note S4 Transfer-printed photonic platform and fundamental characterization

**Figure S6.** Optical images of transfer-printed devices. a) Waveguide arrays for propagation loss measurement using cutback method. b) Fabricated Si-on-LN Mach-Zehnder Modulator (MZM). For simplification of electrode interconnects, half of the spiral waveguides is utilized for tuning and the effective modulation length is calculated with a filling factor. The coupling profile of a straight waveguide was used as the reference to normalize the transmission spectrum for the MZM.

**Figure S7.** Characterization of transfer-printed waveguide. a) Propagation loss measurement using the cut-back method. b) Surface roughness measurement using atomic force microscopy, confirming the prominent uniformness.
Note S5 Theoretical analysis and fitting of Mach-Zehnder interferometer

Figure S8. Schematic of the imbalanced Mach-Zehnder interferometer (MZI). $E_i$ and $E_o$ are the electric field for the input and output respectively; $\beta_0$, $\beta_1$ and $\beta_2$ are different propagation constants respectively and $\alpha$ is absorption coefficient.

For an imbalanced interferometer with length difference $\Delta L$, at the end of two waveguides (at the input to the combiner), the fields are described respectively as:

$$E_{o1} = \frac{E_i}{\sqrt{2}} e^{-i\beta_1 L - \frac{\alpha L}{2}}$$  \hspace{1cm} (Equation S9)

$$E_{o2} = \frac{E_i}{\sqrt{2}} e^{-i\beta_2 L - i\beta_0 \Delta L - \frac{\alpha (L + \Delta L)}{2}}$$  \hspace{1cm} (Equation S10)

Here, the power imbalance of the unbalanced MZI is mainly attributed to propagation loss difference due to the longer length $\Delta L$, defined as:

$$\text{Imb(magnitude)} = \frac{|E_{o2}|^2}{|E_{o1}|^2} = e^{-a\Delta L}$$  \hspace{1cm} (Equation S11)

Without loss of generality, the imbalance can further refer to any power difference between two arms such as imperfect splitting ratio. The output of the combiner is:

$$E_o = \frac{1}{\sqrt{2}} (E_{o1} + E_{o2}) = \frac{E_i}{2} e^{-i\beta_1 L - \frac{\alpha L}{2}} \left(1 + e^{i\Delta \phi - \frac{a \Delta L}{2}}\right)$$  \hspace{1cm} (Equation S12)

where $\Delta \phi(\lambda) = \beta_1 L - (\beta_2 L + \beta_0 \Delta L) = \frac{2\pi \lambda}{\text{FSR}(\lambda)}$ is the phase difference between two arms.

The optical transmission at the output is:

$$T(\lambda) = \frac{|E_o|^2}{|E_i|^2} = \frac{1}{4} e^{-aL} \left[1 + e^{i\Delta \phi - \frac{a \Delta L}{2}}\right]^2 = \frac{1}{4} e^{-aL} \left[1 + 2\sqrt{\text{Imb}} \cos \left(\frac{2\pi \lambda}{\text{FSR}(\lambda)}\right) + \text{Imb}\right]$$ \hspace{1cm} (Equation S13)

For all measured transmission spectra depicted in Figure S9a, we applied a linear fit to the destructive positions or fringes to obtain a linear dispersion estimate of the free spectral range (FSR) as shown in Figure S9b. For each fringe, we extracted a 2-FSR-wide portion of the
spectrum centered on the dip and normalized the constructive intensity to 0 dB, followed by fitting with Equation S13. After that, the imbalances can be obtained from the fitting parameters, plotted in Figure S6d.

**Figure S9.** a) Retrieval of the fringe positions of the measured transmission spectrum. b) Linear fit of the dependence of the free spectral range (FSR) on the wavelength. c) Example fit of normalized spectrum around a single fringe. d) The fitted MZI power imbalance and FSR for depicted wavelength range.
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Reference


