Supplementary Materials for:

An Improved Theoretical Model to Extract the Optical Conductivity of Two-Dimensional Material from Terahertz Transmission or Reflection Spectroscopy

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The derivation of the different orders of the transmitted and reflected fields:

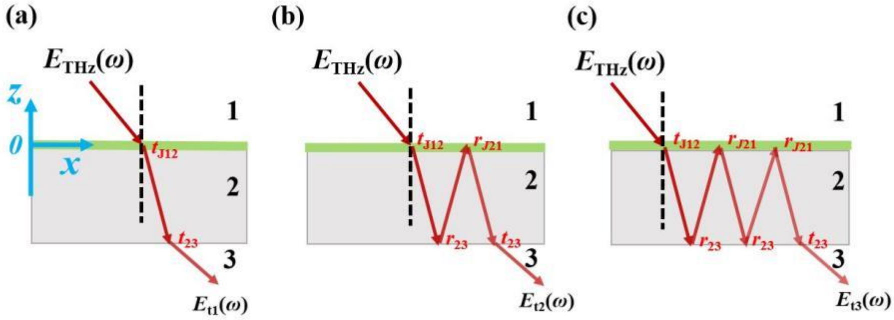

Figure S1. Schematics of the (a) 1st-order, (b) 2nd-order, and (c) 3rd-order transmitted fields.

Firstly, the THz field $E_{\mathrm{THz}}(\omega)$ propagates along a length of $z-L$ in air, where $z-L$ is the distance between the transmitter and receiver. This propagation introduces a phase change in the electric/magnetic field:

$$p_{\mathrm{air}}(\omega, z-L) = exp(-i\tilde{n}_{\mathrm{air}}k_0(z-L)) = e^{-i\delta_{\mathrm{air}}} . \tag{S1}$$

Since the response of the 2D material is treated as a surface current and d is neglected, the phase of the THz wave passing through the 2D material is only changed due to the imaginary part of σ rather than the thickness d. Then, the THz wave enters the substrate (medium 2) and propagates from the upper surface to the bottom surface in z direction. Therefore, this process can induce a phase change associated with $\tilde{n}_2 k_0 L$ in the electric/magnetic field:

$$p_{\mathrm{sam}}(\omega, L) = exp(-i\tilde{n}_2 k_0 L) = e^{-i\delta} . \tag{S2}$$

By considering the transmission coefficients of each interface of the system shown Figure S1(a), the 1st-order transmitted field can be expressed as:

$$\tilde{E}_{\mathrm{t1}}(\omega) = E_{\mathrm{THz}}(\omega) e^{-i\delta_{\mathrm{air}}} t_{J12} e^{-i\delta} t_{23} . \tag{S3}$$

For the 2nd-order transmitted wave, two times of reflection on the upper/bottom interface should be considered in contrast to the 1st-order one, as shown in Figure S1(b). Accordingly, the THz wave passes through the substrate two more times and thereby introduce a phase term of $e^{-i2\delta}$. We can derive the

2nd-order transmitted field by including this phase term into Eq. (S4), which results in the following expression:

$$\tilde{E}_{t2}(\omega)=E_{\mathrm{THz}}(\omega)e^{-i\delta_{\mathrm{air}}}t_{J12}r_{23}r_{J21}e^{-i3\delta}t_{23}\,. \qquad \text{(S4)}$$

Similarly, the 3rd-order transmitted field shown in Figure S1(c) can be obtained as:

$$\tilde{E}_{t3}(\omega)=E_{\mathrm{THz}}(\omega)e^{-i\delta_{\mathrm{air}}}t_{J12}r_{23}^{2}r_{J21}^{2}e^{-i5\delta}t_{23}\,. \qquad \text{(S5)}$$

Considering the iterative process of multiple reflections, the *m*-th-order transmitted field is:

$$\tilde{E}_{tm}(\omega)=E_{\mathrm{THz}}(\omega)e^{-i\delta_{\mathrm{air}}}t_{J12}r_{J23}^{m-1}r_{J21}^{m-1}e^{-i(2m-1)\delta}t_{23}\,. \qquad \text{(S6)}$$

Next, the results of the reflected fields can be obtained easily based on the discussion above and the schematics shown in Figure S2:

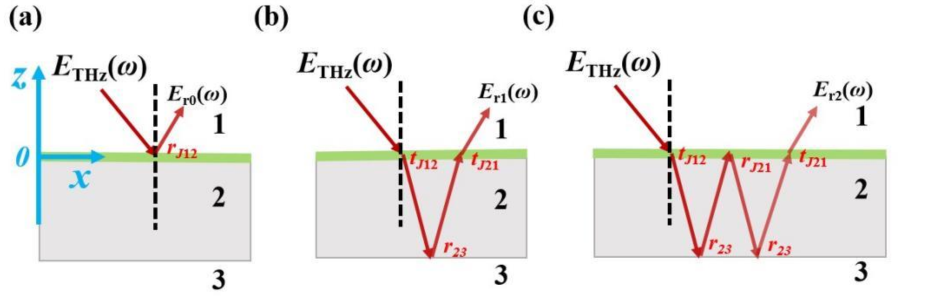

Figure S2. Schematics of the (a) 0-order, (b) 1st-order, and (c) 2nd-order reflected fields.

$$\tilde{E}_{r0}(\omega)=E_{\mathrm{THz}}(\omega)r_{J12}e^{-i\delta_{\mathrm{air}}}\,, \qquad \text{(S7a)}$$

$$\tilde{E}_{r1}(\omega)=E_{\mathrm{THz}}(\omega)t_{J12}r_{23}t_{J21}e^{-i2\delta}e^{-i\delta_{\mathrm{air}}}\,, \qquad \text{(S7b)}$$

$$\tilde{E}_{r2}(\omega)=E_{\mathrm{THz}}(\omega)t_{J12}r_{23}^{2}r_{J21}t_{J21}e^{-i4\delta}e^{-i\delta_{\mathrm{air}}}\,. \qquad \text{(S7c)}$$

Considering the iterative process of multiple reflections, the *m*-th-order reflected field can be expressed as:

$$\tilde{E}_{rm}(\omega)=E_{\mathrm{THz}}(\omega)t_{J12}r_{23}^{m}r_{J21}^{m-1}t_{J21}e^{-i2m\delta}e^{-i\delta_{\mathrm{air}}}\,. \qquad \text{(S8)}$$

Furthermore, by taking the multiple reflections in the slab into account, the total reflection coefficient can be written as follows,

$$\tilde{r}_{\mathrm{total}}(\omega)=r_{J12}+\frac{t_{J12}r_{23}t_{J21}e^{-i2\delta}}{1-r_{J21}r_{23}e^{-i2\delta}}\Bigg/\left(r_{12}+\frac{t_{12}r_{23}t_{21}e^{-i2\delta}}{1-r_{21}r_{23}e^{-i2\delta}}\right). \qquad \text{(S9)}$$