Electronic Supplementary Material (ESI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2022

Electronic Supplementary Information

Two-dimensional natural hyperbolic materials: from polaritons modulation to applications

Guangyi Jia,a Jinxuan Luo,a Huaiwen Wang,a,b Qiaoyun Ma,a Qinggang Liu,c Haitao Dai,d and Reza Asgari,e

aSchool of Science, Tianjin University of Commerce, Tianjin 300134, P. R. China
bTianjin Key Laboratory of Refrigeration Technology, Tianjin University of Commerce, Tianjin 300134, P. R. China
cState Key Laboratory of Precision Measurement Technology and Instruments, Tianjin University, Tianjin 300072, P. R. China
dTianjin Key Laboratory of Low Dimensional Materials Physics and Preparing Technology, School of Science, Tianjin University, Tianjin 300072, P. R. China
eSchool of Physics, Institute for Research in Fundamental Sciences, IPM, Tehran 19395-5531, Iran

Lonrentz model for calculating anisotropic permittivities of HMs

To describe the infrared permittivities of α-MoO₃ and α-V₂O₅ crystals in Fig. 3 in the main article, a three-parameter Lorentz oscillator model is used with

\[ \varepsilon_{ij} = \varepsilon_{ij}^\infty \prod_m \left( \frac{\omega_{LO}^m \omega_{TO}^m}{\omega_{LO}^m - \omega^2 - i\omega \Gamma_{LO}^m} \right)^2 \]

where \( \varepsilon_{ij} \) denotes the principal components of the permittivity tensor, \( \varepsilon_{ij}^\infty \) is the high-frequency dielectric constant. The parameters \( \omega_{LO}^m \) and \( \omega_{TO}^m \) represent the longitude and transverse optical phonon frequencies, respectively. The factor \( \Gamma_{LO}^m \) is the broadening factor of the Lorentzian lineshape. The superscripts \( x, y, \) and \( z \) indicate three principal axes of the crystal along the crystal directions [100], [001], and [010], respectively, and \( m \) is the mode index along three crystal directions. The detailed parameter values utilized in our calculation for α-MoO₃ and α-V₂O₅ are shown in Table S1.
| HMs   | Crystal directions | m | $\omega^L_{\mu m}$ (cm$^{-1}$) | $\omega^T_{\mu m}$ (cm$^{-1}$) | $\Gamma^L_{\mu m}$ (cm$^{-1}$) | $\Gamma^T_{\mu m}$ (cm$^{-1}$) | $\varepsilon_{\mu \mu}$ |
|-------|-------------------|---|-------------------------------|-------------------------------|-------------------------------|-------------------------------|------------------|
| $\alpha$-MoO$_3$ | [100]             | 1 | 972                           | 820                           | 4.0                           | 4.0                           | 4.0              |
|       |                   | 2 | 265.5                         | 261.0                         | 8.0                           | 8.0                           | 8.0              |
|       |                   | 3 | 390.5                         | 303.0                         | 12.2                          | 12.2                          | 12.2             |
|       |                   | 4 | 586.0                         | 411.0                         | 20.0                          | 20.0                          | 20.0             |
|       | [010]             | 1 | 1004                          | 958                           | 2.0                           | 2.0                           | 2.0              |
|       |                   | 2 | 265.5                         | 261.0                         | 8.0                           | 8.0                           | 8.0              |
|       |                   | 3 | 390.5                         | 303.0                         | 12.2                          | 12.2                          | 12.2             |
|       |                   | 4 | 586.0                         | 411.0                         | 20.0                          | 20.0                          | 20.0             |
| $\alpha$-V$_2$O$_5$ | [100]             | 1 | 76.2                          | 72.4                          | 4.2                           | 4.2                           | 4.2              |
|       |                   | 2 | 265.5                         | 261.0                         | 8.0                           | 8.0                           | 8.0              |
|       |                   | 3 | 390.5                         | 303.0                         | 12.2                          | 12.2                          | 12.2             |
|       |                   | 4 | 586.0                         | 411.0                         | 20.0                          | 20.0                          | 20.0             |
|       |                   | 5 | 959.0                         | 767.5                         | 30.0                          | 30.0                          | 30.0             |
|       |                   | 6 | 982.0                         | 980.5                         | 15.0                          | 15.0                          | 15.0             |
|       | [001]             | 1 | 490.0                         | 473.0                         | 15.0                          | 15.0                          | 15.0             |
|       |                   | 2 | 1038.0                        | 975.5                         | 2.5                           | 2.5                           | 2.5              |
|       |                   | 3 | 842.5                         | 506.5                         | 18.0                          | 18.0                          | 18.0             |
|       | [010]             | 1 | 225.0                         | 212.0                         | 7.5                           | 7.5                           | 7.5              |
|       |                   | 2 | 312.5                         | 284.0                         | 10.2                          | 10.2                          | 10.2             |
|       |                   | 3 | 842.5                         | 506.5                         | 18.0                          | 18.0                          | 18.0             |

Table S1: Parameter values used for calculating the anisotropic permittivities of $\alpha$-MoO$_3$ and $\alpha$-V$_2$O$_5$