



# Machine Learning–Enhanced Tunable Terahertz Metasurface Sensor with a Hybrid Multi-Resonator Architecture for High-Sensitivity Amino Acid Detection

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## Abstract

Accurate amino acid detection is essential for biomedical diagnostics, clinical monitoring, and biochemical research; however, conventional analytical techniques are often constrained by complex sample preparation, high operational costs, and limited real-time capability. Terahertz (THz) metasurface sensors provide a promising label-free and non-ionizing alternative, yet their performance is frequently hindered by weak light–matter interaction and design trade-offs between sensitivity and fabrication feasibility.

In this work, a hybrid THz metasurface sensor is proposed, integrating graphene, gold (Au), silver (Ag), copper (Cu), and tungsten disulfide (WS<sub>2</sub>) within a hierarchical multi-resonator configuration comprising square, circular ring, and L-shaped resonators fabricated on a SiO<sub>2</sub> substrate. The proposed architecture exploits synergistic plasmonic–dielectric coupling and strong near-field confinement to enhance sensitivity to refractive index perturbations induced by amino acid analytes, while maintaining a geometrically simplified structure to ensure manufacturability.

Numerical simulations demonstrate excellent sensing performance, achieving a maximum sensitivity of 1000 GHz/RIU, a peak figure of merit (FOM) of 50 RIU<sup>-1</sup>, and a strong linear relationship ( $R^2=0.96243$ ) between resonance frequency shift and analyte refractive index. Furthermore, machine learning (ML) models are employed to predict and optimize sensor behavior, yielding near-perfect accuracy ( $R^2>0.9995$ ) for variations in graphene chemical potential (0.1–0.9 eV) and circular resonator dimensions (5.5–7.5  $\mu\text{m}$ ). The proposed integration of hybrid materials, multi-resonator metasurface design, and ML-driven optimization effectively addresses key challenges in THz biosensing, enabling rapid, sensitive, and scalable amino acid detection for both point-of-care diagnostics and advanced biochemical research.

**Keywords** Terahertz metasurface sensor · Machine learning · Amino acid detection · Tunable plasmonics · Hybrid materials · Refractive index sensing

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