Supplementary Information *for* Anomalous optical response of graphene on hexagonal boron nitride substrates

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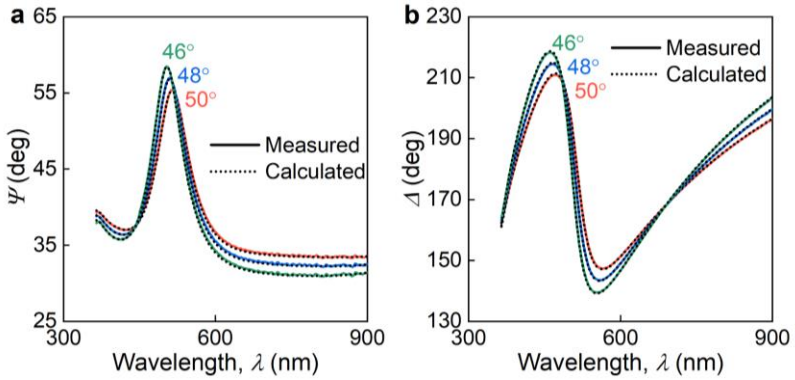

Figure S1: Ellipsometric parameters Ψ **(a)** and Δ **(b)** of monolayer graphene on SiO_2/Si substrate at three incident angles of 46°, 48°, 50°. Solid (dashed) lines represent the measured (calculated) cases.

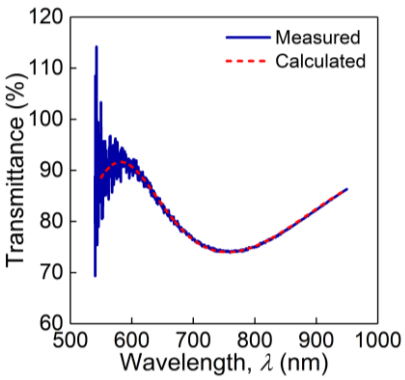

Figure S2: Micro-transmittance spectra of *h*BN on glass substrate. Solid (dashed) line represents the measured (calculated) case.

We performed a set of *ab initio* calculations to study the effects of *h*BN influence on optical response of monolayer graphene varying their interlayer distances from 3.38 Å (relaxed geometry) down to 2.66 Å with 0.24 Å step. For each of the boundary cases the extinction coefficients are shown in Figure S3. Notably, at 2.66 Å, those show animal behavior in transverse direction at the wavelength range from 200 to 800 nm. Here, we employed a simple model of layered structure and ignored in-plane lattice mismatch between graphene and *h*BN in-plane parameters. For calculations, we considered 2×2 supercell of graphene and *h*BN to decrease mechanical stresses during geometry minimization. The total lattice mismatch did not exceed 0.8 % for both graphene and *h*BN. Geometry optimization of graphene/*h*BN heterostructures were carried out through density functional theory (DFT) [S1, S2] within the generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) parameterization for exchange-correlation functional[S3] implemented in VASP package[S4-S6].

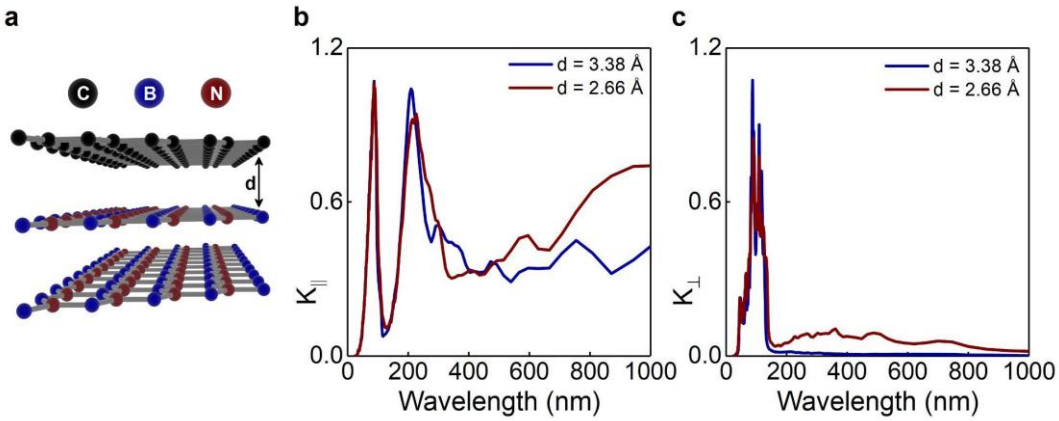

Figure S3: (a) Schematic illustration of monolayer graphene on top of bilayer *h*BN used for *ab initio* evaluations. Evaluated extinction coefficient for **(b)** *ab*-plane and **(c)** *c*-axis. Calculations were carried out for different distances between the graphene and *h*BN, at *d* = 2.66 Å (red line) and *d* = 3.38 Å (blue line), which corresponds to the relaxed geometry.

Van der Waals interactions were taken into account through Grimme correction[S7]. The cutoff energy of plane waves was set to 520 eV. The sampling of the Brillouin zone was done with a uniform *k*-points grid of 6×6×1. The extinction coefficient was calculated using the superposition of Lorentz oscillators to simulate the complex frequency-dependent dielectric function. The real part was determined *via* the Kramers-Kronig relations, while the imaginary part was found by summing over unfilled states[S8]. The extinction coefficient was expressed through the complex dielectric function $\varepsilon_1 + i\varepsilon_2$ as

$$K(\lambda) = \sqrt{\frac{\sqrt{(\varepsilon_1^2 - \varepsilon_2^2)} - \varepsilon_1}{2}}$$

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