Supporting Information (SI)/ **Modulating the electro-optical properties of doped C3N monolayer and graphene bilayer via mechanical strain and pressure**

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Computational details for optical properties calculations

In the random phase approximation, the imaginary part of the interband dielectric permittivity is given by [1]:

$$\mathrm{Im}\,\varepsilon_{\alpha\beta}(\omega)=\frac{4\pi^2e^2}{\Omega}\lim_{q\to 0}\frac{1}{|q|^2}\sum_{c,v,k}2w_k\delta(\varepsilon_{ck}-\varepsilon_{vk}-\omega)\times\langle u_{ck+e_\alpha q}|u_{vk}\rangle\langle u_{ck+e_\beta q}|u_{vk}\rangle^{*} \quad (1)$$

where q is the Bloch vector of the incident wave, w_k is the **k**-point weight and the band indices c and v are restricted to the conduction and the valence band states, respectively. By using the $\mathrm{Im}\,\varepsilon_{\alpha\beta}(\omega)$, one can determine the corresponding real part via the Kramers–Kronig relations:

$$\mathrm{Re}\,\varepsilon_{\alpha\beta}(\omega)=1+\frac{2}{\pi}P\int_0^{\infty}\frac{\omega'\,\mathrm{Im}\,\varepsilon_{\alpha\beta}(\omega')}{(\omega')^2-\omega^2+i\eta}d\omega' \quad (2)$$

where P denotes the principle value and η is the complex shift. By taking into account the contribution of intraband transitions for metals [1], it is obtained that:

$$\mathrm{Im}\,\varepsilon_{\alpha\beta}^{[intra]}(\omega)=\frac{\Gamma\omega_{pl,\alpha\beta}^2}{\omega(\omega^2+\Gamma^2)} \quad (3)$$

$$\mathrm{Re}\,\varepsilon_{\alpha\beta}^{[intra]}(\omega)=1-\frac{\omega_{pl,\alpha\beta}^2}{\omega(\omega^2+\Gamma^2)} \quad (4)$$

In these equations ω_{pl} is the plasma frequency and Γ is the life time broadening:

$$\omega_{pl}^2=\frac{n_e e^2}{\varepsilon_0 m^{*}} \quad (5)$$

where n_e is the number density of electrons, e is the electric charge, m^* is the effective mass of the electron. The adsorption coefficient determined as:

$$a_{\alpha\beta}(\omega)=\frac{2\omega k_{\alpha\beta}(\omega)}{c} \quad (6)$$

where $k_{\alpha\beta}$ is imaginary part of the complex refractive index and c is the speed of light in vacuum, known as the extinction index. It is given by the following relations

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$$k_{\alpha\beta}(\omega)=\sqrt{\frac{|\varepsilon_{\alpha\beta}(\omega)-\mathrm{Re}\,\varepsilon_{\alpha\beta}(\omega)|}{2}} \quad (7)$$

The reflectivity is given by

$$R_{ij}(\omega)=\frac{(n-1)^2+k^2}{(n+1)^2+k^2} \quad (8)$$

where *n* and *k* are real and imaginary parts of the complex refractive index, which are known as the refractive index and the extinction index, respectively.

References

[1] F. Wooten, **Optical Properties of Solids**, Academic press (2013).

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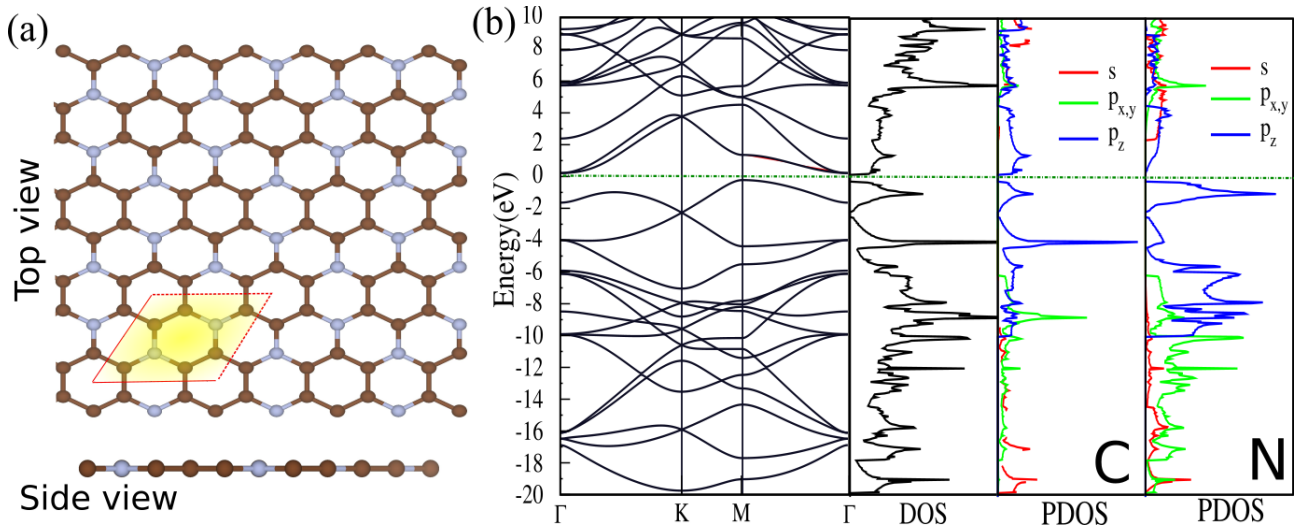

Fig. S1. (a) Atomic structure, electronic and (b) electronic band structure with corresponding density of state (DOS) and partial DOS (PDOS) of C3N monolayer. The zero of energy is at Fermi-level.

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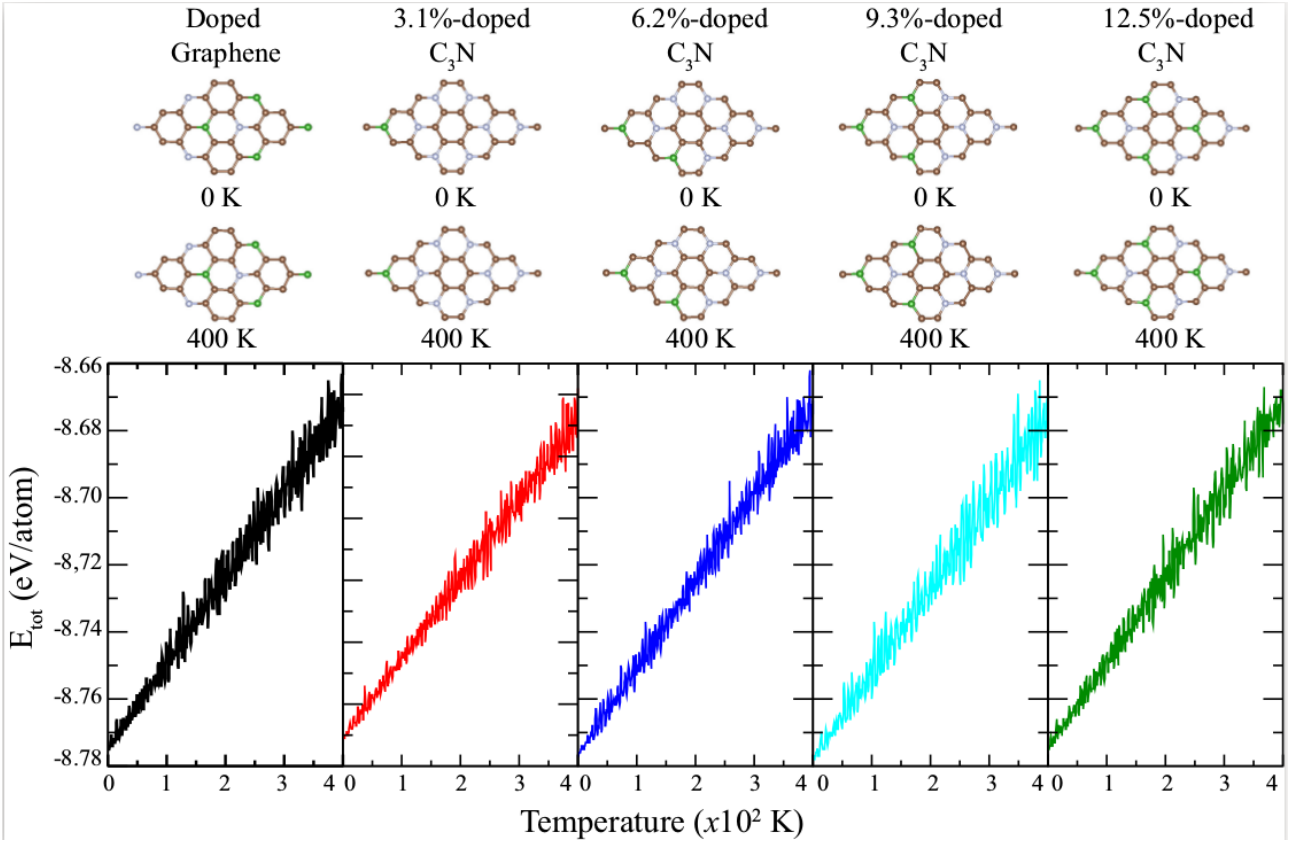

Fig. S2. The ab-initio molecular dynamics (AIMD) simulations of pristine and B-doped C3N monolayer with different concentrations.

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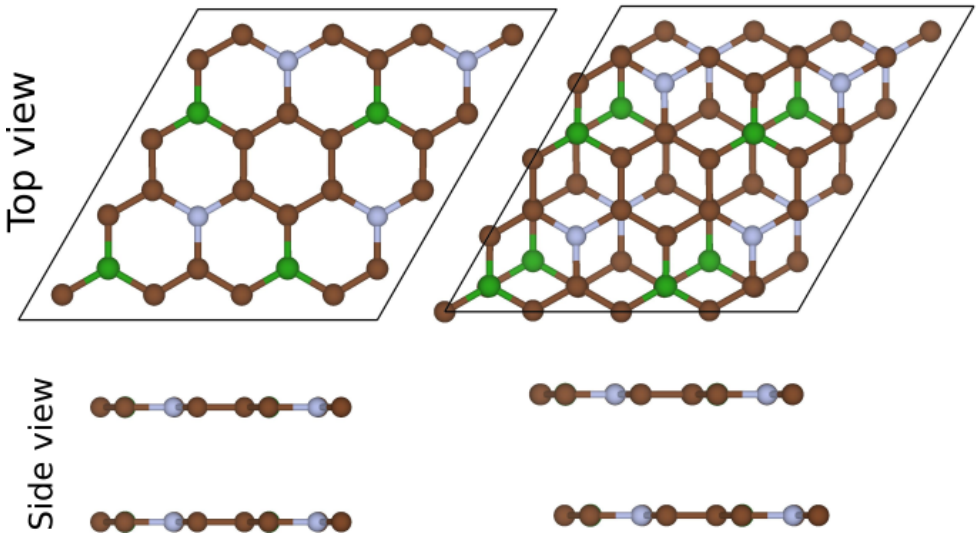

Fig. S3. Top and side views of AA (left) and AB (right) stacking arrangements of B/N-doped graphene bilayer.

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