Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information (SI)

Effect of adsorption and substitutional B doping at different concentrations on the electronic and magnetic properties of BeO monolayer: A First-principles study

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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]:

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

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:

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

where P denotes the principle value and η is the complex shift.

The adsorption coefficient determined as:

$$a_{\alpha\beta}(\omega) = \frac{2\omega k_{\alpha\beta}(\omega)}{c} \quad (3)$$

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

$$k_{\alpha\beta}(\omega) = \sqrt{\frac{\left|\varepsilon_{\alpha\beta}(\omega) - \mathrm{Re}\varepsilon_{\alpha\beta}(\omega)\right|}{2}} \quad (4)$$

The reflectivity is given by

$$R_{ij}(\omega) = \frac{n - 1^2 + k^2}{n + 1^2 + k^2} \quad (5)$$

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.

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References

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

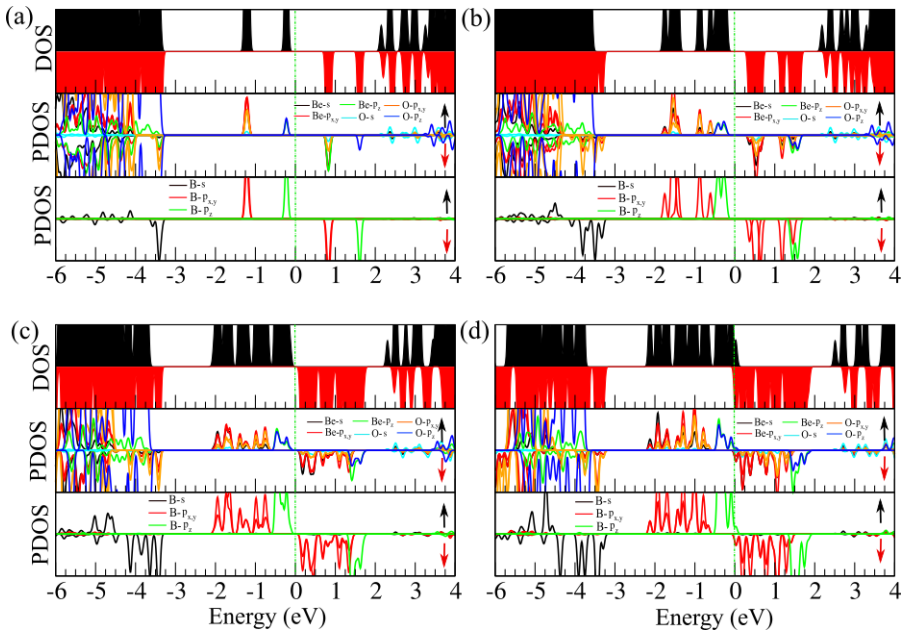

Figure S1. DOS and PDOS of B adsorbed BeO monolayer for different concentrations. The zero of energy is at Fermi-level.

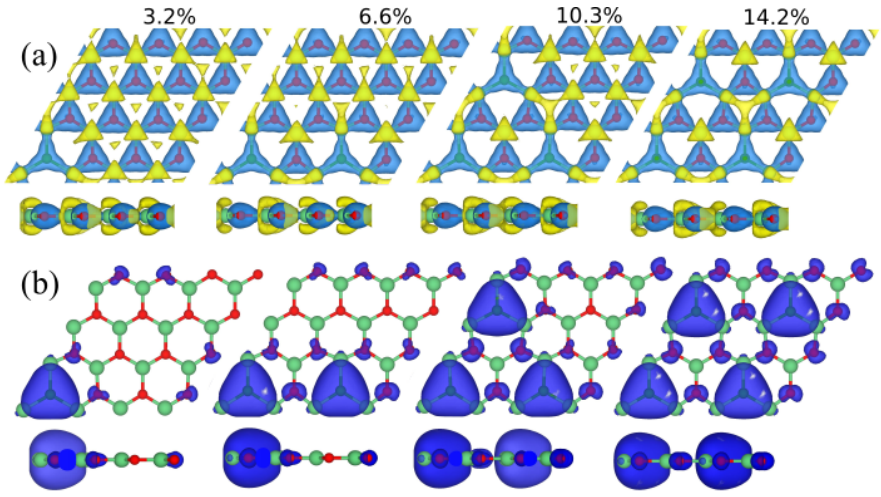

Figure S2. Difference charge and (b) difference spin densities of B doped BeO monolayer for different concentrations. Red (blue) color indicate high (low) electron density.

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