The emerging metal-ion-coordinated black phosphorus nanosheets and black phosphorus quantum dots with excellent stabilities

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Part S1. Analysis of theoretical calculation results

The interactions between metal ions with BP structures belong to the bonding combination, and the calculated adsorption energy is the bonding energy. After theoretical calculations, $E_{\text{Total–Zn}}$ is –2.04 eV. The adsorption energy is negative and indicates that Zn ions can be adsorbed on BP structures. The adsorption energies (–2.87~–6.42 eV) derived from other metal ions adsorbed on BP structures are higher than that of Zn ions adsorbed on BP structures. In addition, the adsorption energy (–39.26 eV) from the non-bonding combination of Zn ions on BP structures is dramatically higher than that from the bonding combination of metal ions on BP structures. The calculated results of adsorption energies indicate that Zn ions can be easily adsorbed on BP structures through bonding combination, when compared to other metal ions. The calculated adsorption energy from bonding combination is lower than that from non-bonding combination. Consequently, Zn ions can serve as the preferred metal ions to be easily adsorbed on BP structures through bonding combination. The resultant Zn@BPNSs and Zn@BPQDs are expected to show highly colloidal, structural and optical stabilities rationally.

Element	Adsorption energy (eV)
Zn	-2.04
Ag	-2.87
Cu	-3.02
Fe	-4.92
Mn	-3.87
Co	-6.42
Zn (Non-Bonding)	-39.26

Fig. S1. The adsorption energies of various types of metal element ions adsorbed on BP structures according to theoretical calculations.

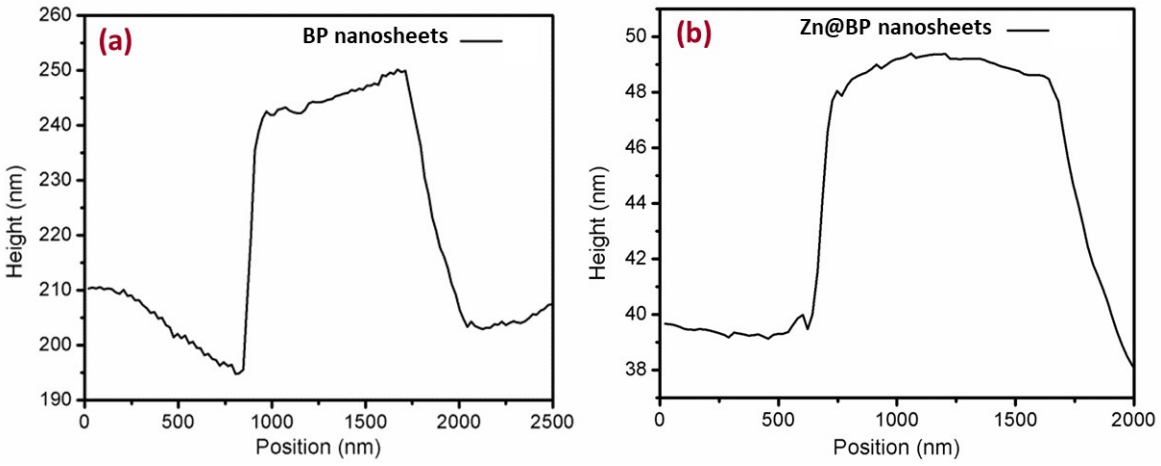

Fig. S2. The height profiles of the exfoliated bare BP nanosheets (a) and Zn@BP nanosheets (b) on basis of AFM images of bare BP nanosheets (Fig. 2l–n) and Zn@BP nanosheets (Fig. 2o–q) in the TEXT.

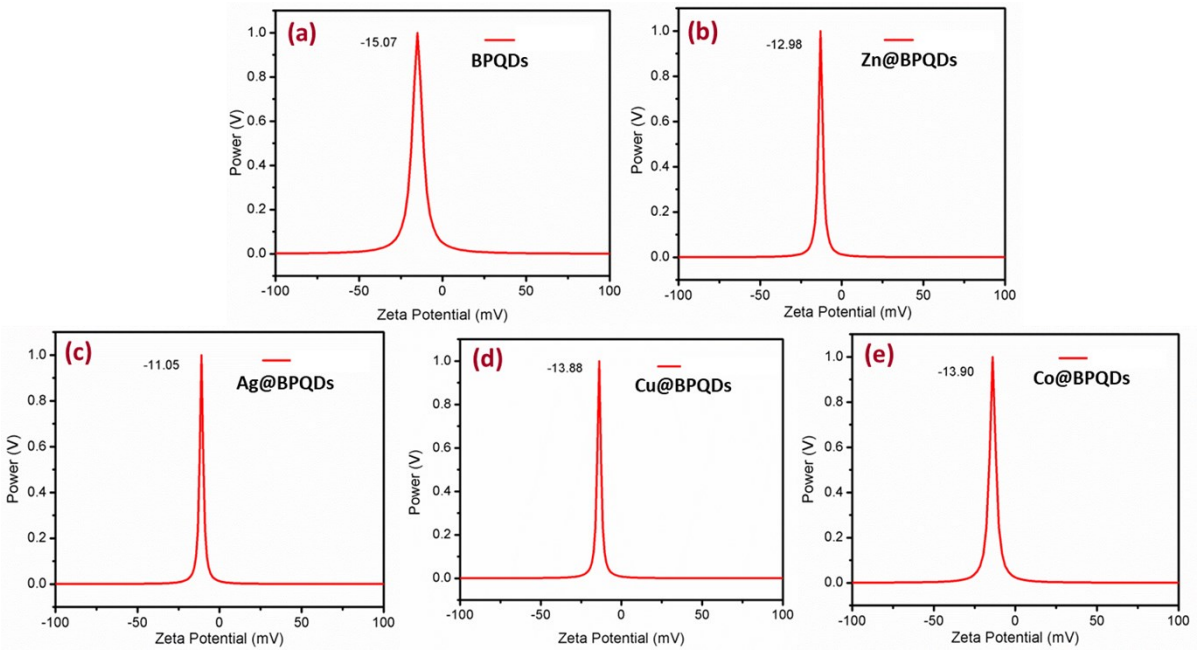

Fig. S3. Zeta potential distributions and average Zeta potentials of the prepared BPQDs, Zn@BPQDs, Ag@BPQDs, Cu@BPQDs and Co@BPQDs, respectively.

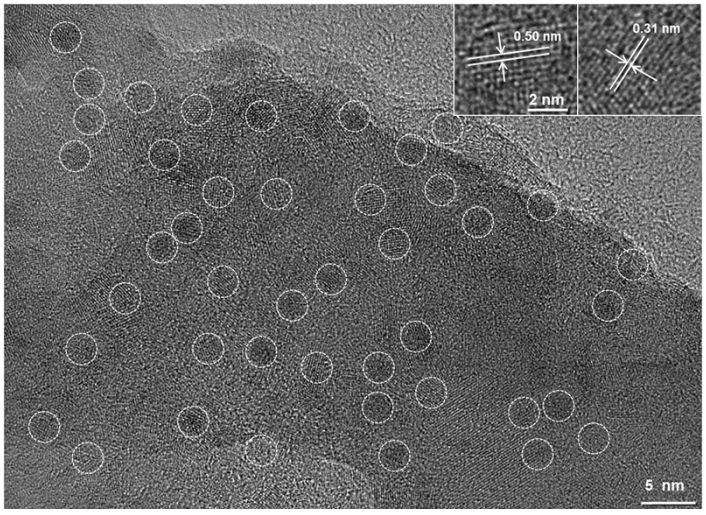

Fig. S4. TEM images and the inserted HR–TEM images of the prepared Zn@BPQDs.

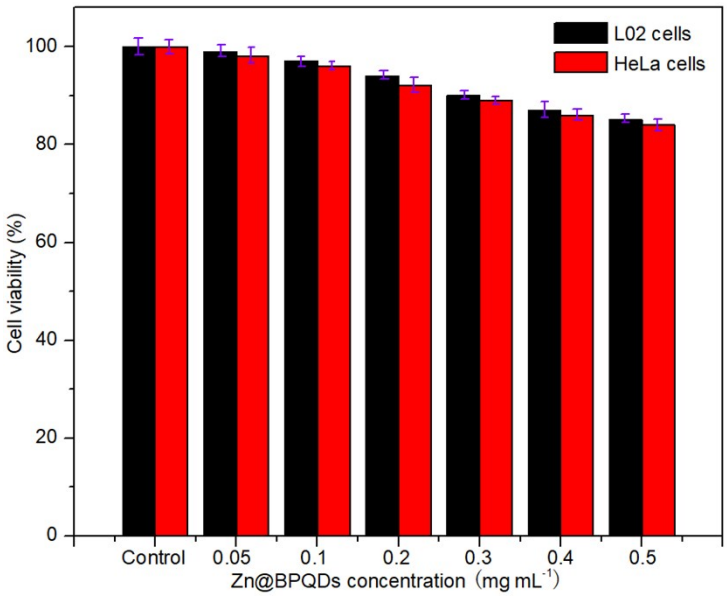

Fig. S5. The viabilities for L02 cells and HeLa cells, with incubation for 48 h in the PBS (10 mM, pH 7.4) aqueous dispersions containing the prepared Zn@BPQDs at different existing concentrations.