Supplementary information

Defect Physics of Intrinsic Point Defects in $BiPO_4$ Photocatalyst: A Hybrid Functional Study

Hongchun Zheng [a], Jincheng Wang [a], Bo Kong [a]*, Xiang Xu [a], Min zhang [a], Wentao Wang [b]*

a. School of Physics and Astronomy, China West Normal University, Nanchong 637002, China;

b. Guizhou Provincial Key Laboratory of Computational Nano-Material Science, Guizhou Education University, Guiyang, 550018, China;

* Corresponding Authors, E-mail: xihuakb@163.com (B. K.); wuli8@163.com(W.W).

Table S1. The total energies (eV) and magnetic moment (μ_B) of the supercell containing a defect in $BiPO_4$ with spin polarization or without spin polarization setting.

	Total energy		magnetic moment
	without spin polarization	with spin polarization	
V_{Bi}^{0}	-1305.40166700	-1305.45471561	0.8924
V_{Bi}^{1-}	-1301.52076614	-1301.52702633	0.5080
V_{Bi}^{2-}	-1297.53500802	-1297.54509022	0.5358
V_{Bi}^{3-}	-1293.51427516	-1293.51739581	0.0000
Bi_i^{0}	-1314.42076588	-1314.55717601	1.0000
Bi_i^{1+}	-1322.31448209	-1322.30646094	0.0000
Bi_i^{2+}	-1328.82282799	-1328.96225845	1.0000
Bi_i^{3+}	-1336.14536442	-1336.14528181	-0.0000

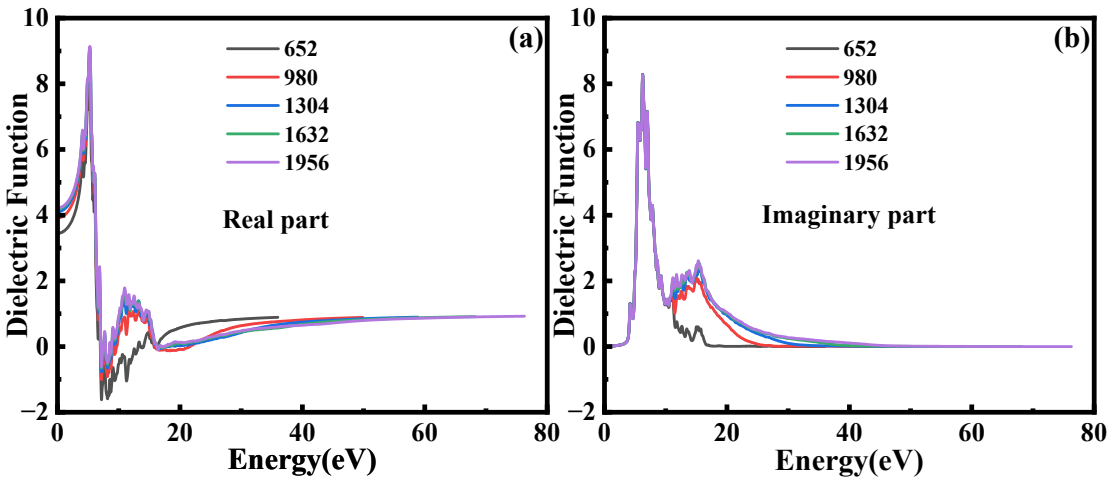

Fig. S1. Differences in the NBANDS parameter settings in the input file lead to variations in the

pure supercell dielectric function; (a) and (b) represent the variations in the real and imaginary parts, respectively. Where the black line in the figure indicates that NBANDS is the default value determined in the HSE results via VASP, the red line indicates that NBANDS is 1.5 times the default value, the blue line shows that NBANDS is 2 times the default value, the green line indicates that NBANDS is 2.5 times the default value, and the purple line indicates that NBANDS is 3 times the default value.

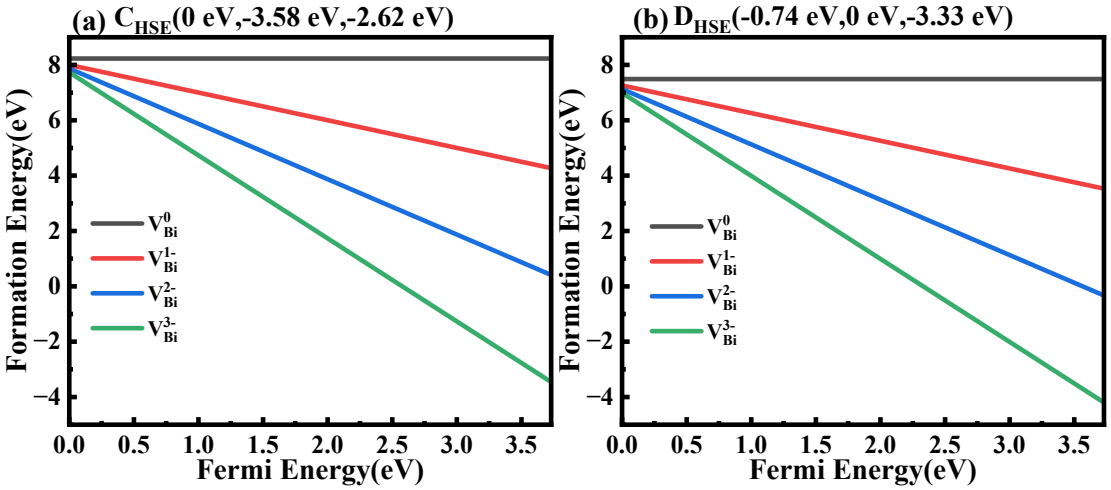

Fig. S2. The variation of the formation energies of different valence Bi vacancies in the range of Fermi energy levels, as exemplified by the C and D chemical potential points in Fig. 1, are shown in (a) and (b), respectively.

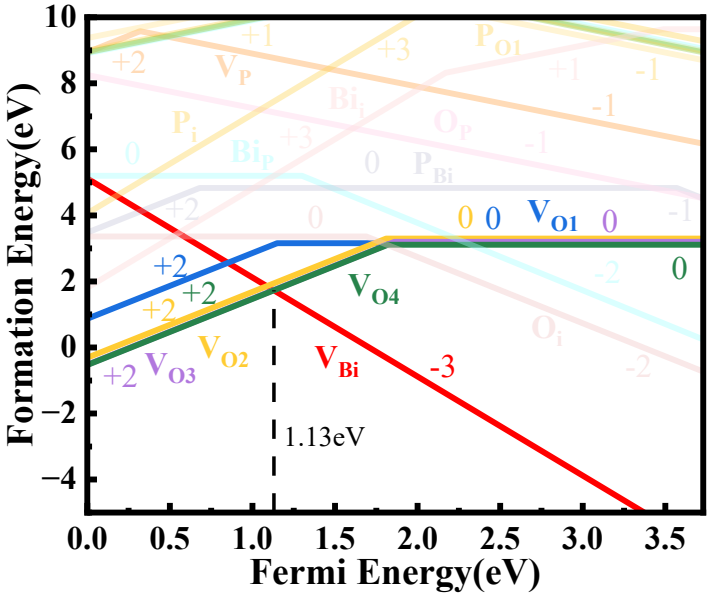

Fig. S3. The variation of HSE formation energy with Fermi energy level for various intrinsic point defects in $BiPO_4$ in different charge states with a representative chemical potential point E_{HSE} ($\Delta\mu_{Bi}$, $\Delta\mu_P$, $\Delta\mu_O$ are -2.61, -5.52, -1.49 eV respectively) in the middle part of the phase diagram (chemical potential reachable range) of $BiPO_4$.

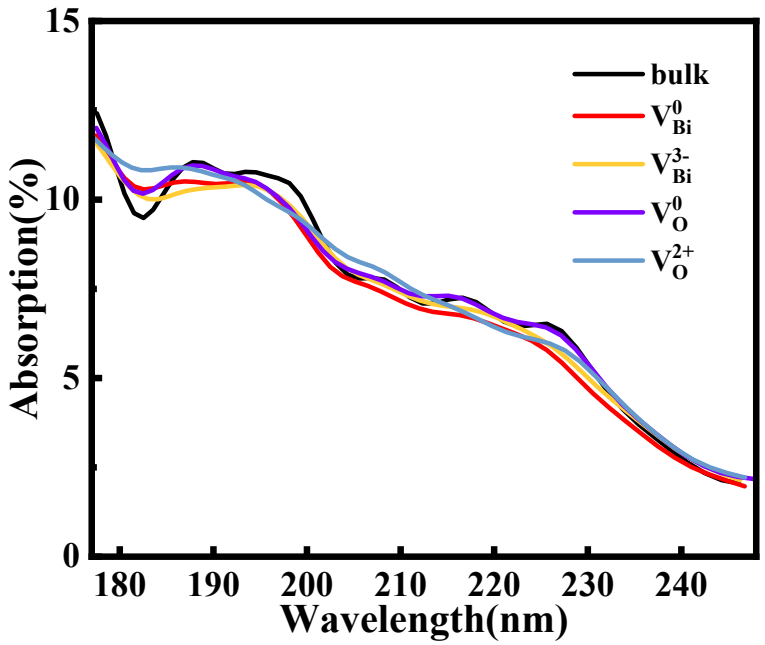

Fig. S4. The optical absorption curves of the supercell with the Bi vacancy or O vacancy in different charge states in $BiPO_4$ via HSE calculations.