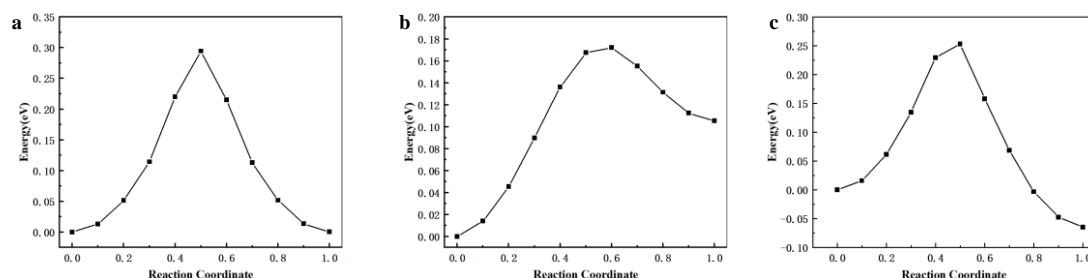# Supporting Information

# Polarons formation and transport in Bi$_2$WO$_6$ studied by DFT+U and hybrid functional approaches

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**Fig. S1** (a) The energy curves for the hole polaron transfer from O$_3$ to O$_5$ site. (b) The energy curves for the hole polaron transfer from O$_4$ to O$_2$ site. (c) The energy curves for the hole polaron transfer from O$_2$ to O$_5$ site.

**Table S1.** The magnetization of each intermediate in the transfer along path calculated by DFT+U approach

| Single point | $m_{O_3}$:$m_{O_5}$/$m_{O_{tol.}}$ | $m_{O_4}$:$m_{O_2}$/$m_{O_{tol.}}$ | $m_{O_2}$:$m_{O_5}$/$m_{O_{tol.}}$ |
|---|---|---|---|
| 0 | 0.002:0.696/0.848 | 0.087:0.705/0.898 | 0.000:0.696/0.848 |
| 0.1 | 0.002:0.684/0.850 | 0.116:0.691/0.913 | 0.000:0.682/0.850 |
| 0.2 | 0.004:0.670/0.082 | 0.158: 0.672/0.934 | 0.000:0.666/0.853 |
| 0.3 | 0.005: 0.651/0.856 | 0.221:0.641/0.961 | 0.000:0.643/0.856 |
| 0.4 | 0.018: 0.544/0.849 | 0.314:0.590/ 0.990 | 0.006:0.598/ 0.860 |
| 0.5 | 0.190: 0.301/ 0.873 | 0.430:0.503/1.010 | 0.160:0.468/0.959 |
| 0.6 | 0.558: 0.020/0.851 | 0.533:0.391/1.021 | 0.603:0.062/0.948 |
| 0.7 | 0.649: 0.019/0.857 | 0.604:0.284/1.004 | 0.652:0.033/0.930 |
| 0.8 | 0.670: 0.013/0.854 | 0.646:0.207/0.982 | 0.673:0.023/0.918 |
| 0.9 | 0.684: 0.009/0.851 | 0.672: 0.154/0.963 | 0.691:0.017/0.907 |
| 1.0 | 0.696:0.006/0.848 | 0.691:0.118/0.950 | 0.705:0.012/0.898 |

$m_{O_2}$, $m_{O_3}$, $m_{O_4}$, $m_{O_5}$ are the magnetization on the O$_2$ , O$_3$, O$_4$, O$_5$ site. $m_{O_{tol.}}$ is the total magnetization on O sites. For the transfer from O$_3$ site to O$_5$ site, O$_4$ site to O$_2$ site, and O$_2$ site to O$_5$, the hole polaron transfer distance is 2.807 Å, 2.787 Å and 3.171 Å, the activation energy $\Delta G^*$ is 0.294 eV, 0.172 eV and 0.253 eV, the calculated mobility is 1.58 ×10$^{-6}$ cm$^2$V$^{-1}$s$^{-1}$, 1.83×10$^{-4}$ cm$^2$V$^{-1}$s$^{-1}$,and 1.00×10$^{-5}$ cm$^2$V$^{-1}$s$^{-1}$ .