1. The "OPV.txt" contains 515 data points (as shown in Table S3 and S4) for correlation analysis and machine learning (Columns 1 to 7: *E*g, Δ*E*DA, Δ*E*ST, *V*OC, *J*SC, FF, and PCE).
2. Combined with the "OPV.txt" and Scikit-Learn, the "OPVpredict\_loo.py" and "OPVpredict\_cv.py" can reproduce the results reported in Figure 4 and 5 and Table S5.