

Experimental EA (eV)

−3.0
−3.2
−3.4
−3.6
−3.8
−4.0
−4.2

$y = 0.528 x + 0.907$
 $R^2=0.64$
RMSE=5.066

−9.5

−9.0

−8.5

−8.0

sTDA-xTB LUMO (eV)

