

Experimental EA (eV)

-3.0
-3.2
-3.4
-3.6
-3.8
-4.0
-4.2

$y = 0.621x + 1.865$
 $R^2 = 0.631$
RMSE=5.287

-9.5

-9.0

-8.5

-8.0

GFN2 LUMO (eV)

