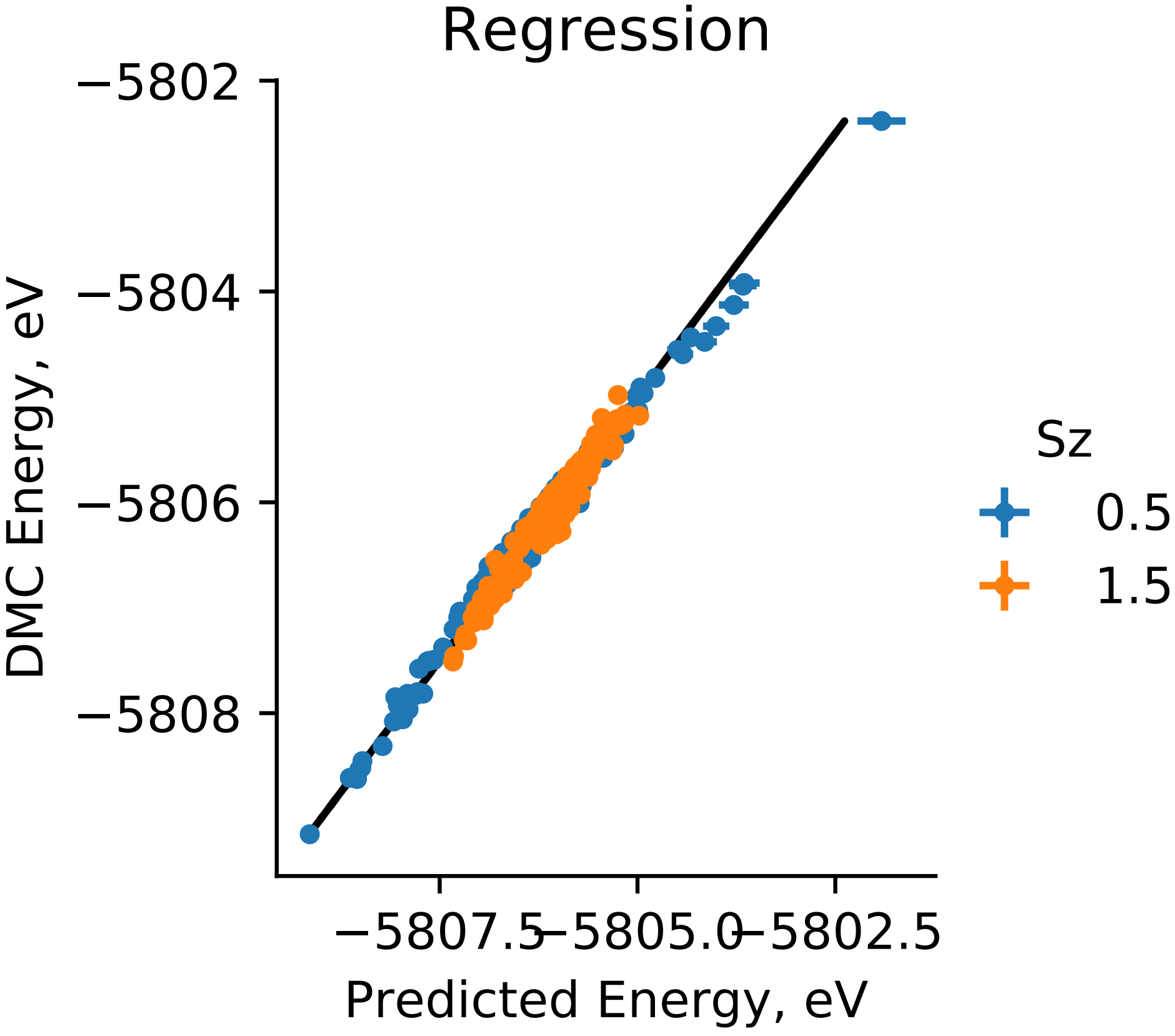
Regression
−5802
−5804
−5806
−5808
DMC Energy, eV
−5807.5
−5805.0
−5802.5
Predicted Energy, eV
Sz
0.5
1.5