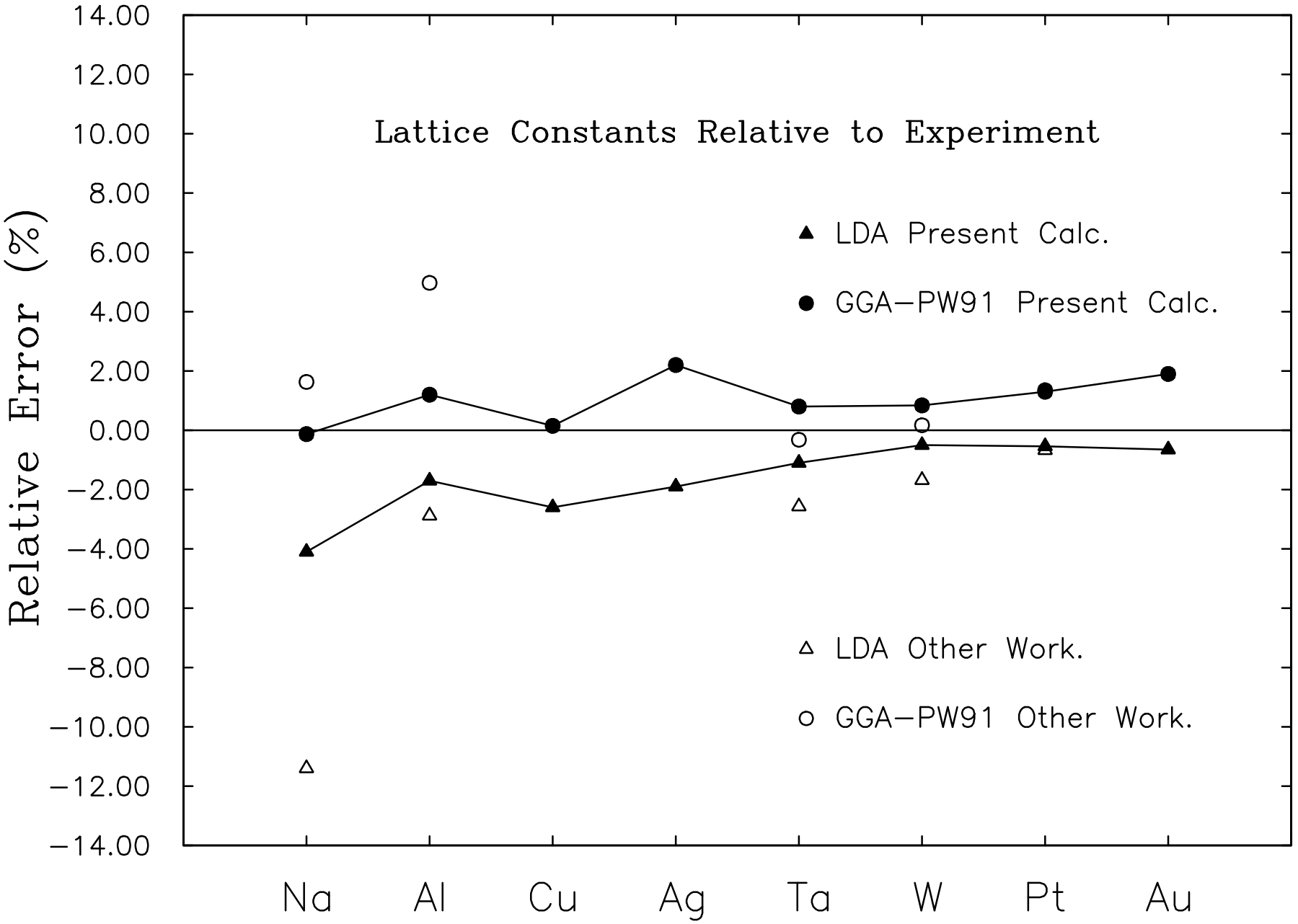
Lattice Constants Relative to Experiment
Relative Error (%)
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
−2.00
−4.00
−6.00
−8.00
−10.00
−12.00
−14.00
Na
Al
Cu
Ag
Ta
W
Pt
Au
LDA Present Calc.
GGA−PW91 Present Calc.
LDA Other Work.
GGA−PW91 Other Work.