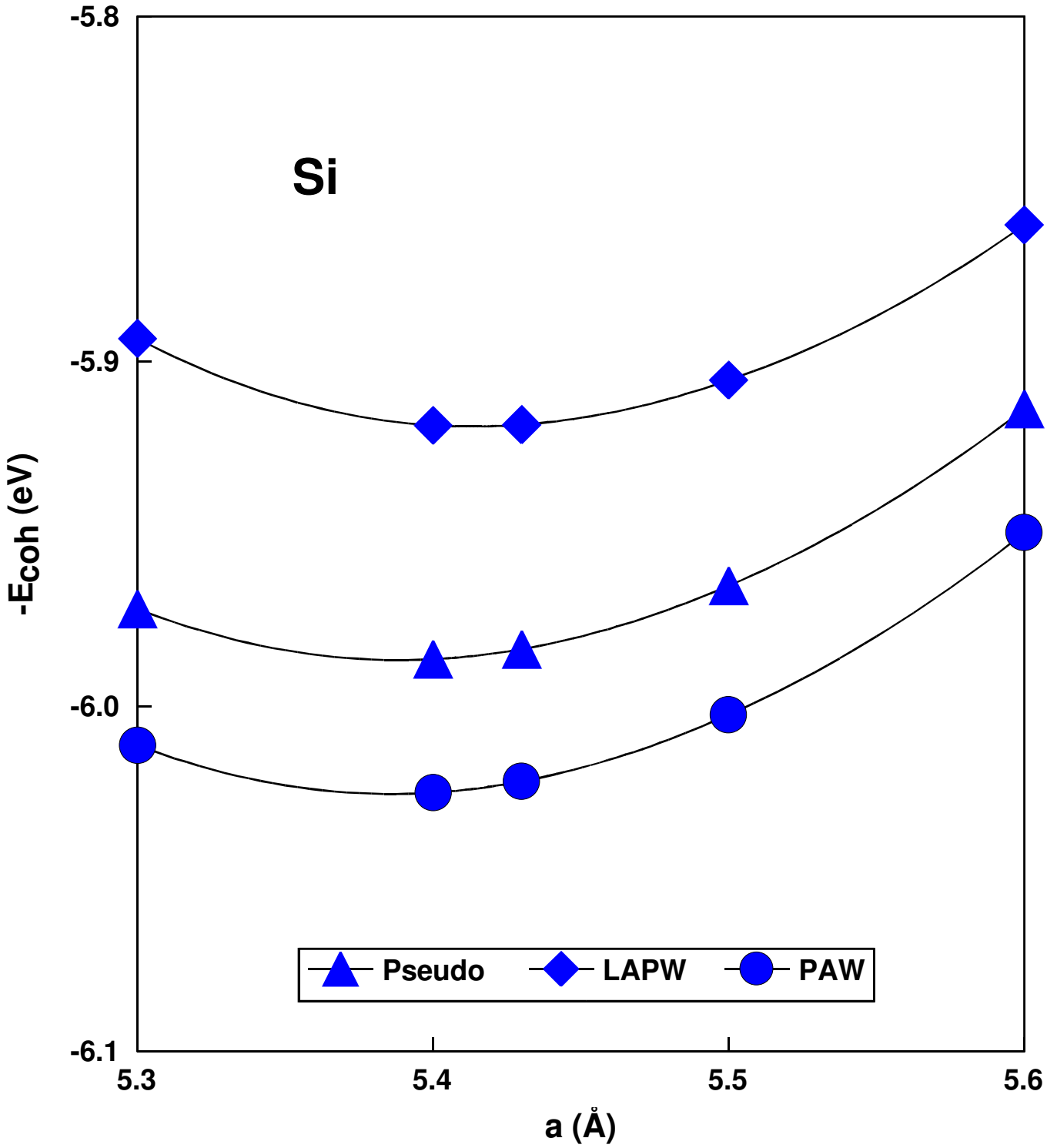
Si
-5.8
-5.9
-6.0
-6.1
-Ecoh (eV)
5.3
5.4
5.5
5.6
a (Å)
Pseudo
LAPW
PAW