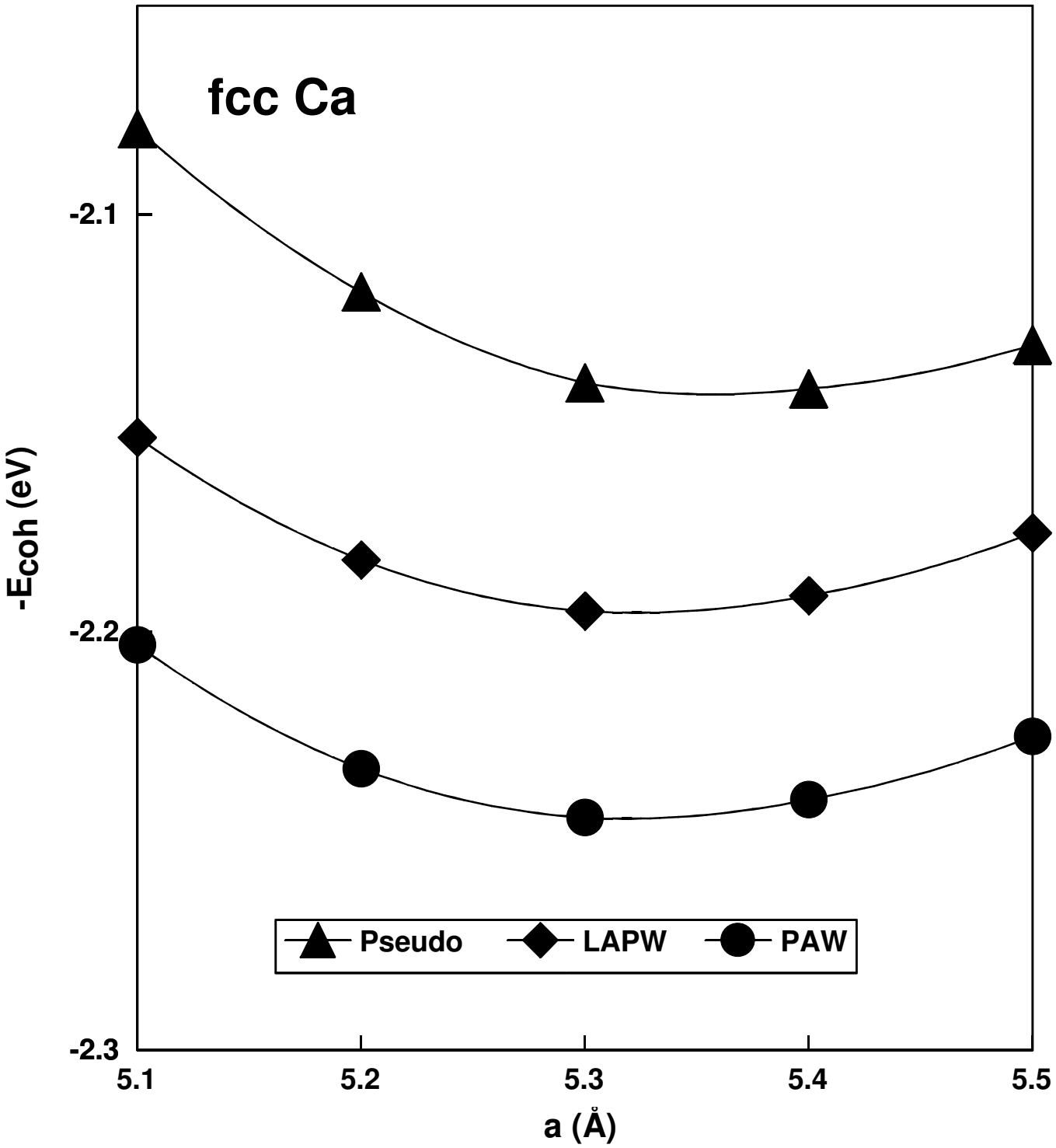
fcc Ca
-2.1
-2.2
-2.3
-Ecoh (eV)
5.1
5.2
5.3
5.4
5.5
a (Å)
Pseudo
LAPW
PAW