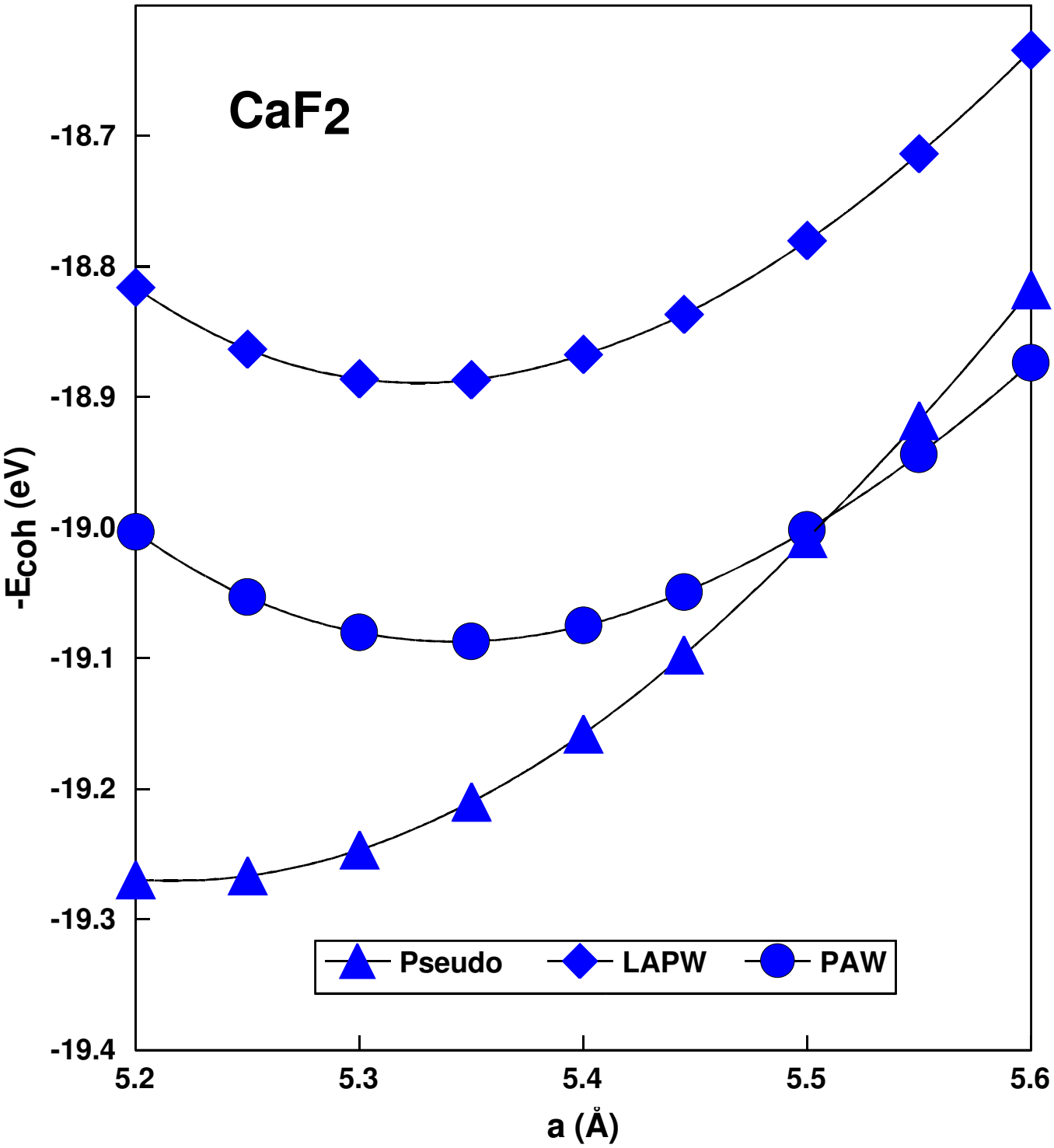
CaF2
-18.7
-18.8
-18.9
-19.0
-19.1
-19.2
-19.3
-19.4
-Ecoh (eV)
5.2
5.3
5.4
5.5
5.6
a (Å)
Pseudo
LAPW
PAW