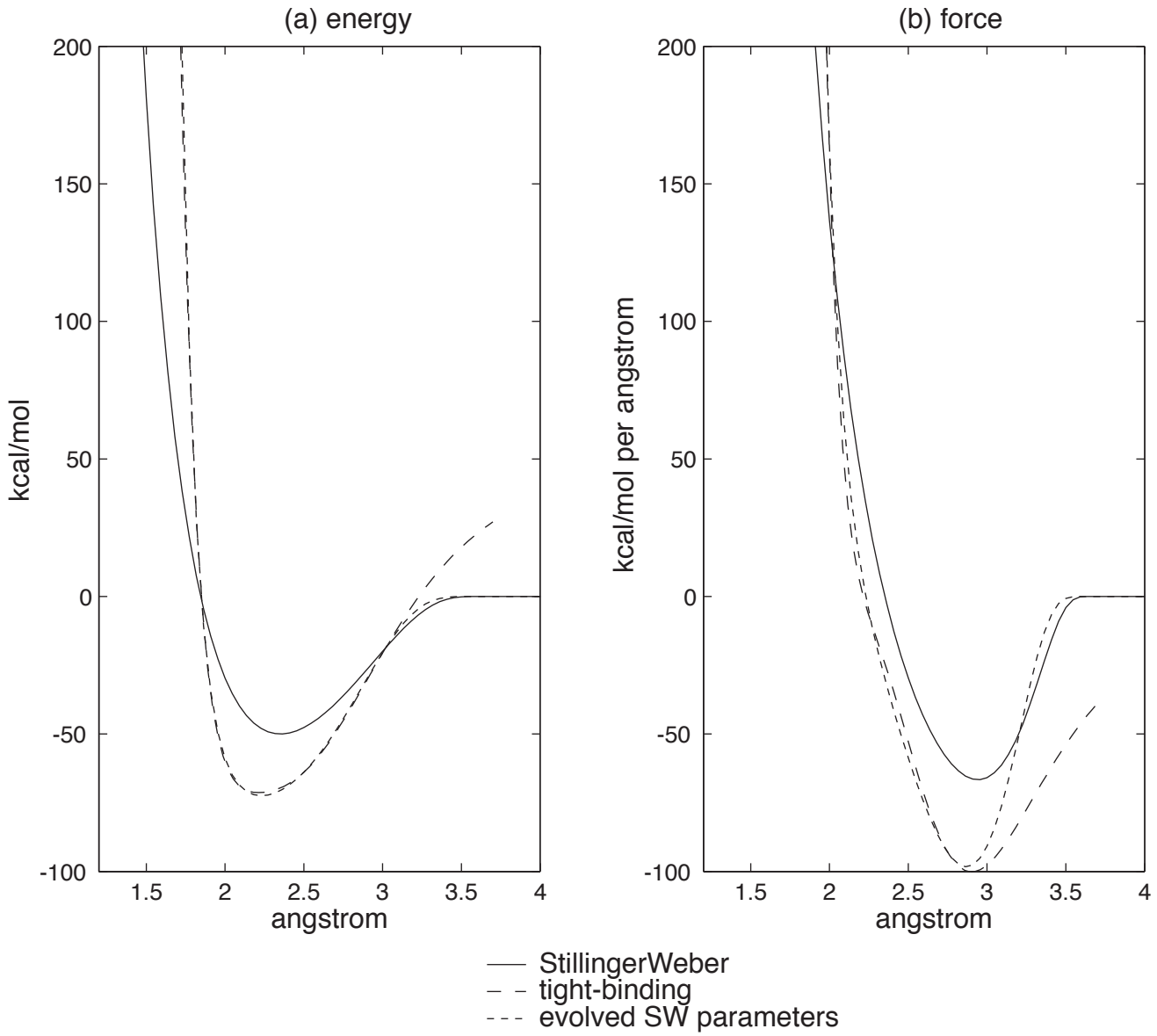
Figure 4


(a) energy
(b) force
kcal/mol
kcal/mol per angstrom
angstrom
angstrom
200
150
100
50
0
-50
-100
1.5
2
2.5
3
3.5
4
StillingerWeber
tight-binding
evolved SW parameters