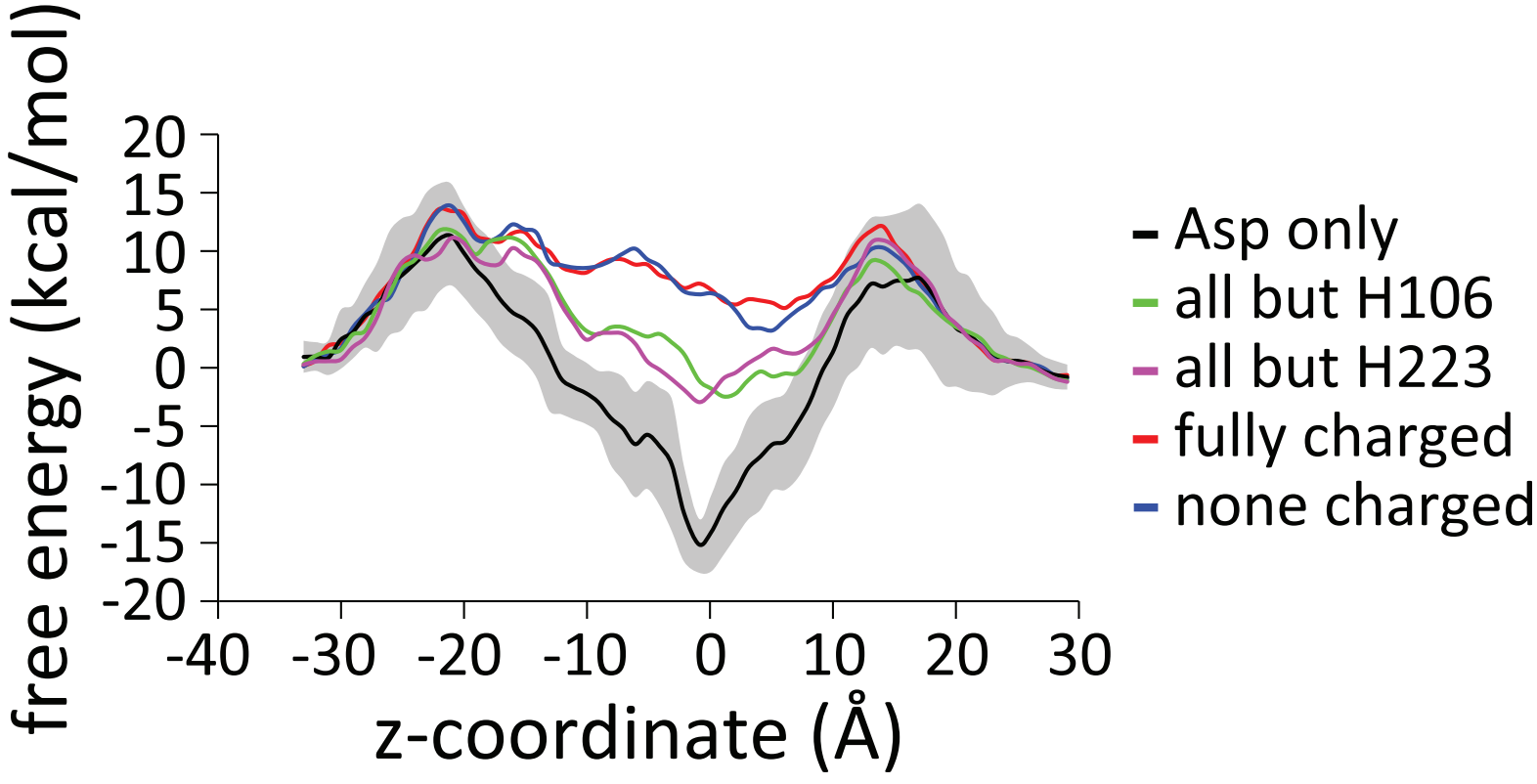
free energy (kcal/mol)
20
15
10
5
0
-5
-10
-15
-20
-40
-30
-20
-10
0
10
20
30
z-coordinate (Å)
Asp only
all but H106
all but H223
fully charged
none charged