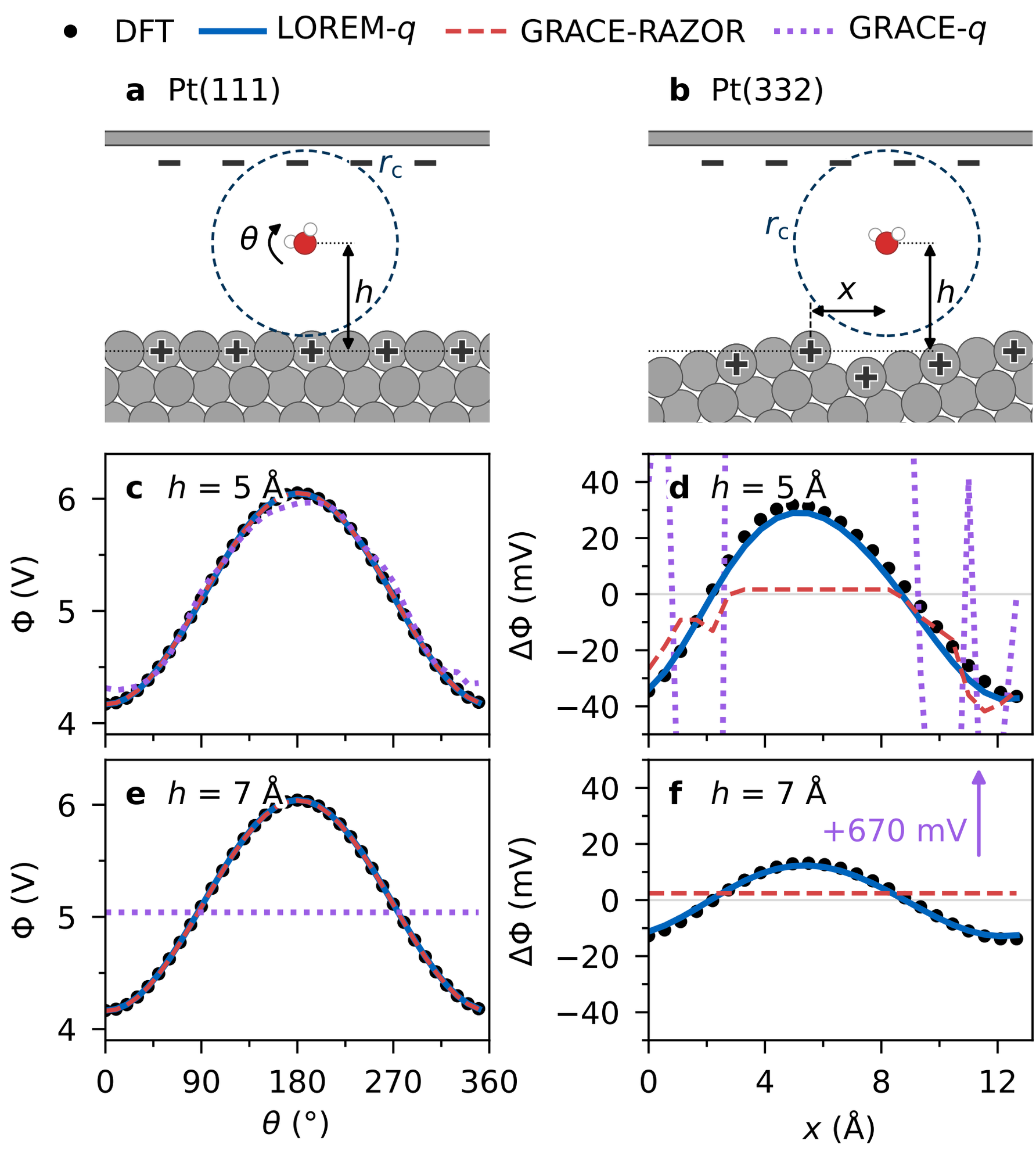

DFT
LOREM-q
GRACE-RAZOR
GRACE-q
a Pt(111)
b Pt(332)
r_c
θ
h
x
c h = 5 Å
d h = 5 Å
e h = 7 Å
f h = 7 Å
+670 mV
Φ (V)
ΔΦ (mV)
θ (°)
x (Å)
0
90
180
270
360
4
8
12
40
20
−20
−40
4
5
6