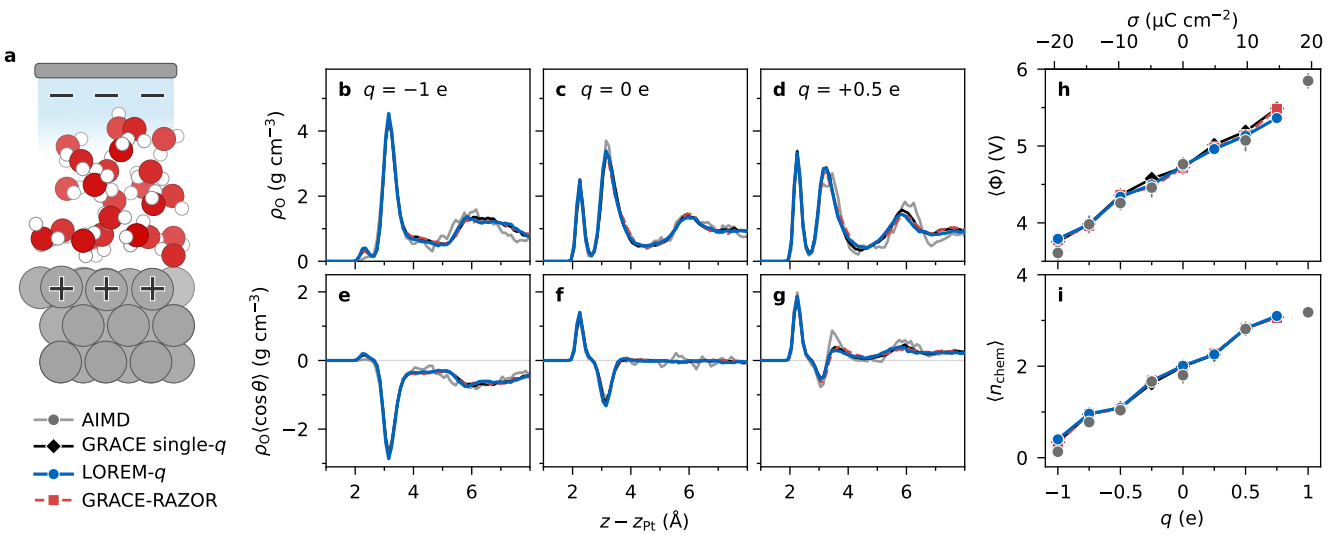

a
AIMD
GRACE single-q
LOREM-q
GRACE-RAZOR
b q = −1 e
c q = 0 e
d q = +0.5 e
e
f
g
ρO (g cm−3)
ρO(cos θ) (g cm−3)
z − zPt (Å)
σ (μC cm−2)
h
i
⟨Φ⟩ (V)
⟨nchem⟩
q (e)