# *Lisa Eggart*

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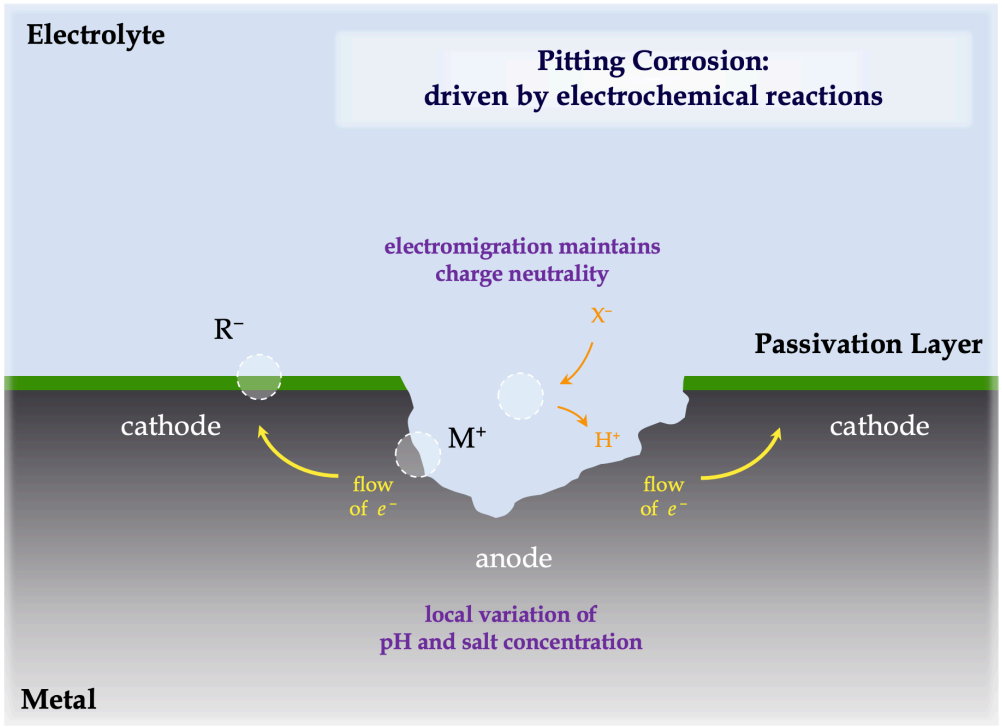
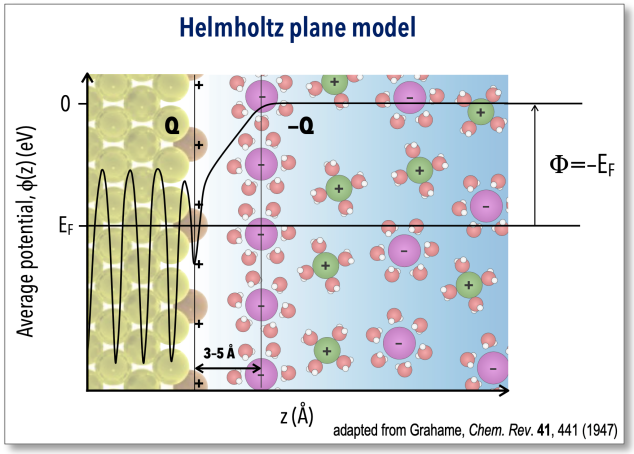
## Research Topic: computational model of the onset of electrochemical pitting corrosion



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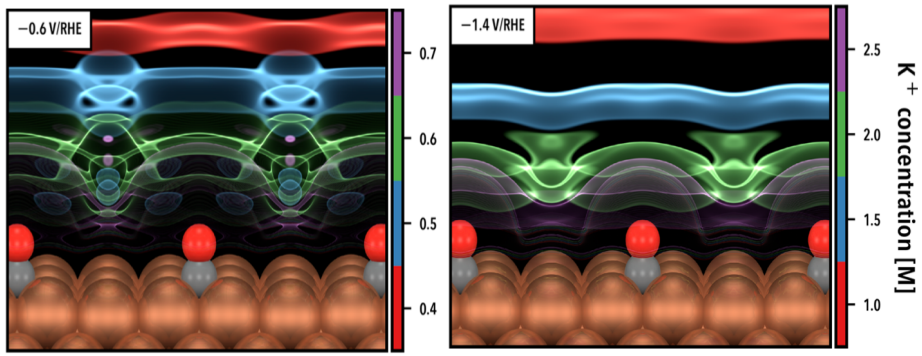
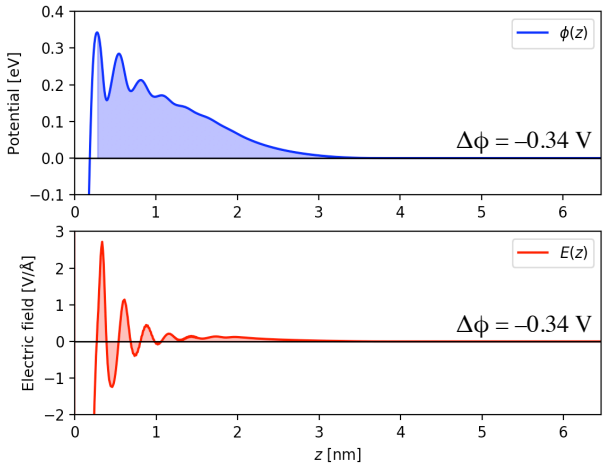
# Computational Challenge: interfacial solvent-modeling




Weitzner et al., *The Journal of Physical Chemistry Letters* (2020)




ESM-RISM
atomic density derived from classical force fields and can be used for potential referencing

$$\Delta\phi = \phi(z_2) - \phi(z_1) = -\int_{z_1}^{z_2} E(z)dz$$

# This Week's Goal: increased computational fluency