Questions:

1. What is the subject of this work?

A: Understanding the selectivity of CO2 reduction on Sn

2. Why Sn?

A: Earth-abundant; high selectivity for formate

3. What are the previous theories on the selectivity of CO2 reduction on Sn?

A: (1) One electron transfer to radical; protonation of radical and further reduction

(2) From intermediates like *COOH and *OCHO on surfaces

Questions:

4. How do the authors find the descriptor for formate formation on various metals?

A: Plotting partial current densities against the computed *COOH and *OCHO energies; the correaltion with *OCHO gives a Volcano plot.

5. What is the explanation for the selectivity of CO2 reduction on Sn?

A: Near optimal *OCHO binding energy.

6. What is a potential major limitation/complication for this type of correlation?

A: The correlation is based on thermodynamic considerations; kinetic phenomenon can alter the selectivity.