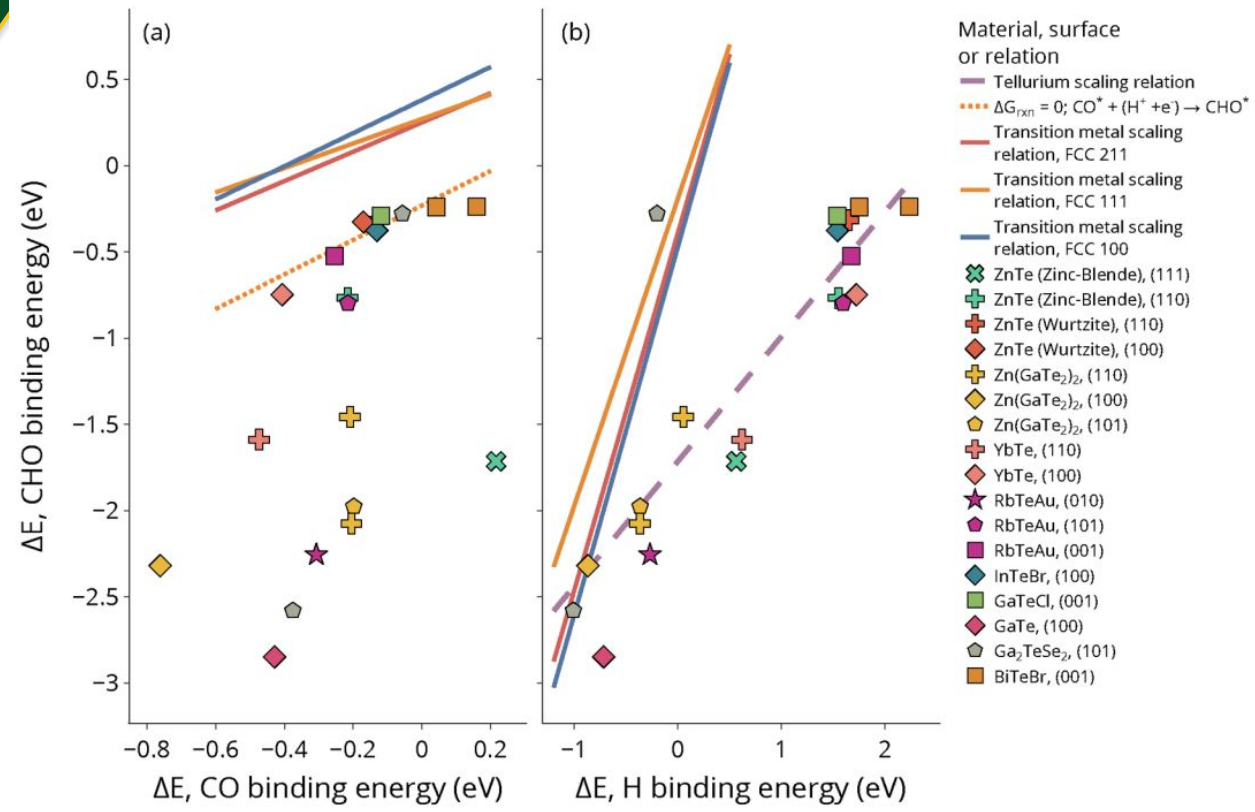
Data-Driven Investigation of Tellurium-Containing Semiconductors for CO2 Reduction: Trends in Adsorption and Scaling Relations



Scientific Achievement:

Calculated over 650 chemisorption energies on 11 tellurium-containing semiconductors.

Significance and Impact:

- Found scaling relation between *CHO and *H for both charge transfer and chemisorption energy that is absent with *CO. Explained relationship through orbital contribution to bonding using Crystal Orbital Hamiltonian Population analysis.
- Calculated that on these materials *CHO is quite stabilized, thus if *CO can be adsorbed these materials could produce potential CO_2RR products. Unfortunately most of these materials do not adsorb CO2.
- Found elemental specific design rules: in general, Zn, Yb, Rb, Br, and Cl sites tend to have less competition with hydrogen evolution reaction.

Research details:

- 650+ chemisorption energies using Density Functional Theory. Calculations performed with rPBE functional and plane-wave basis set. Calculations performed in VASP.

Siron, M. Andriuc, O. Persson, A. P., ACS JPCC (2022), https://pubs.acs.org/doi/10.1021/acs.jpcc.2c04810

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