Supplementary Information

Uniting Activity Design Principles of Anode Catalysts for Direct Liquid Fuel Cells

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Supplementary Note 1. Calculation of thermodynamic values for liquid fuels

The thermodynamic values of liquid fuels were calculated from the oxidation reaction and values from standard tables from the NIST Standard Reference Database[1] and chemical handbooks.[2–4]. The standard Gibbs free energy of reaction $\Delta G^{\circ}_{r,i}$ of species i at 25 °C was calculated from the oxidation half-reaction through

$$\Delta G^{\circ}_{r,i} = \sum_{j} \nu_i \Delta_f G^{\circ}_i$$

where ν_i is the stoichiometric coefficient for species i and $\Delta_f G^{\circ}_i$ is the standard Gibbs free energy of formation for species i.

The standard oxidation potential E° was calculated using the relation

$$E_i^{\circ} = -\frac{\Delta G^{\circ}_{r,i}}{-zF}$$

where z is the number of electrons transferred per mole of liquid fuel oxidation and F is Faraday's constant (96485 C mol^{-1}).

The overall cell potential was calculated assuming that the oxygen reduction reaction (ORR) occurs at the cathode with the following equation,

$$E^{\circ}_{cell,i} = E^{\circ}_{ORR} - E^{\circ}_i$$

The specific energy of liquid fuel i (S_i) was then calculated using

$$S_i = \frac{-zFE^{\circ}_i}{M_i}$$

where M_i is the molar mass of liquid fuel i. Using the density of liquid fuel i (ρ_i) at room temperature and atmospheric pressure, the energy density D_i was calculated by

$$D_i = \rho_i S_i$$

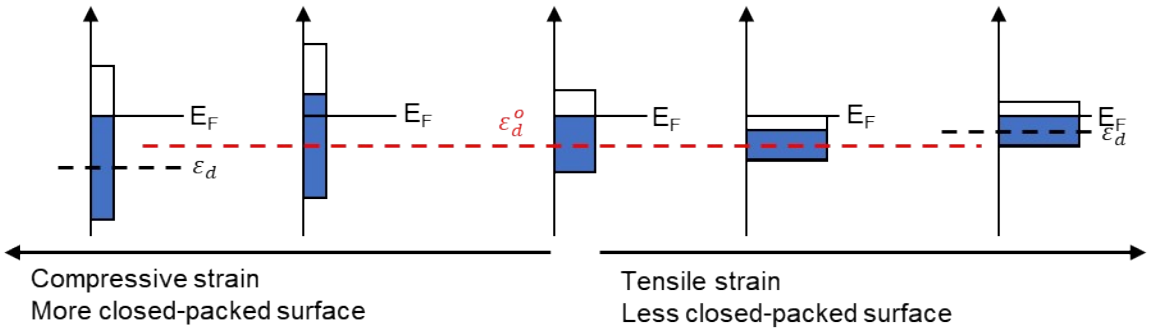

Figure S1. Schematic demonstrating the shifts in d-band center due to changes in the electronic structure of a metal surface.

References

1. *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*. (National Institute of Standards and Technology, 2018).
2. *CRC Handbook of Chemistry and Physics*. (CRC Press, 2011).
3. *Perry's Chemical Engineers' Handbook*. (McGraw-Hill Education, 2008).
4. *Chemical Properties Handbook: Physical, Thermodynamics, Environmental, Transport, Safety and Health Related Properties for Organic and Inorganic Chemicals*. (McGraw-Hill Education, 1999).