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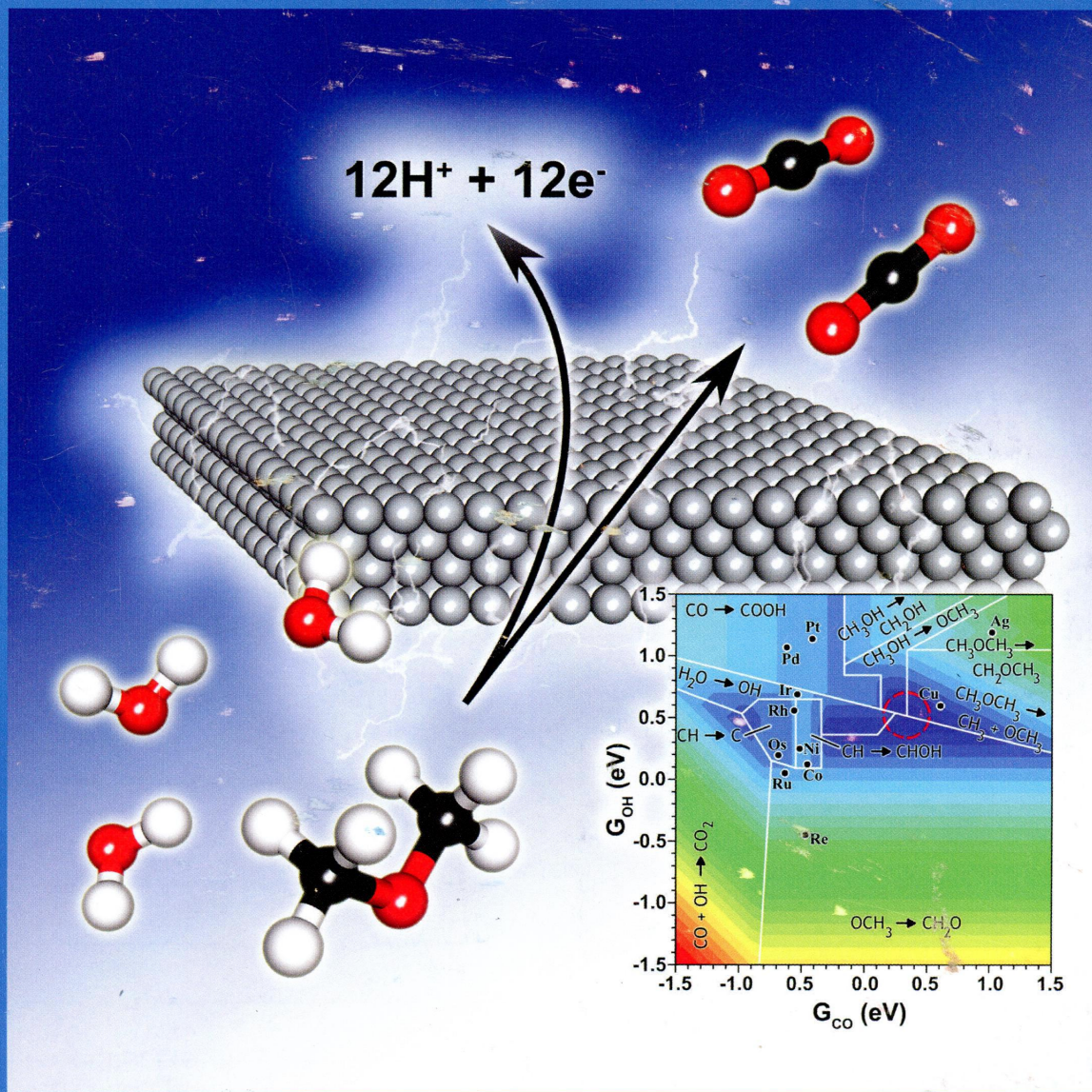
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# THE JOURNAL OF PHYSICAL CHEMISTRY

# C

Catalyst Design  
from First-Principles:  
Dimethyl Ether  
Electro-Oxidation  
(see page 24199)



ENERGY CONVERSION AND STORAGE, OPTICAL AND ELECTRONIC DEVICES,  
INTERFACES, NANOMATERIALS, AND HARD MATTER



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**ON THE COVER:** Catalyst design from first-principles: dimethyl ether electro-oxidation. Theoretical phase diagram (lower right) showing the free energy of reaction for the most energetically difficult step as a function of reactivity descriptors: free energies of adsorbed CO and OH. Monometallic closepacked surfaces are indicated for reference. The blue color indicates the region of highest activity (circled in red), while the region colored in red is the least active. See page 24199

## Feature Article

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[dx.doi.org/10.1021/jp505919x](https://doi.org/10.1021/jp505919x)

**First-Principles Mechanistic Analysis of Dimethyl Ether Electro-Oxidation on Monometallic Single-Crystal Surfaces**

Jeffrey A. Herron, Peter Ferrin, and Manos Mavrikakis\*

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**Local Interfacial Migration of Clay Particles within an Oil Droplet in an Aqueous Environment**

Kyongok Kang,\* J. S. Hong, and J. K. G. Dhont

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