Identifying Promising Ionic Liquids for Electrochemical CO_2 reduction

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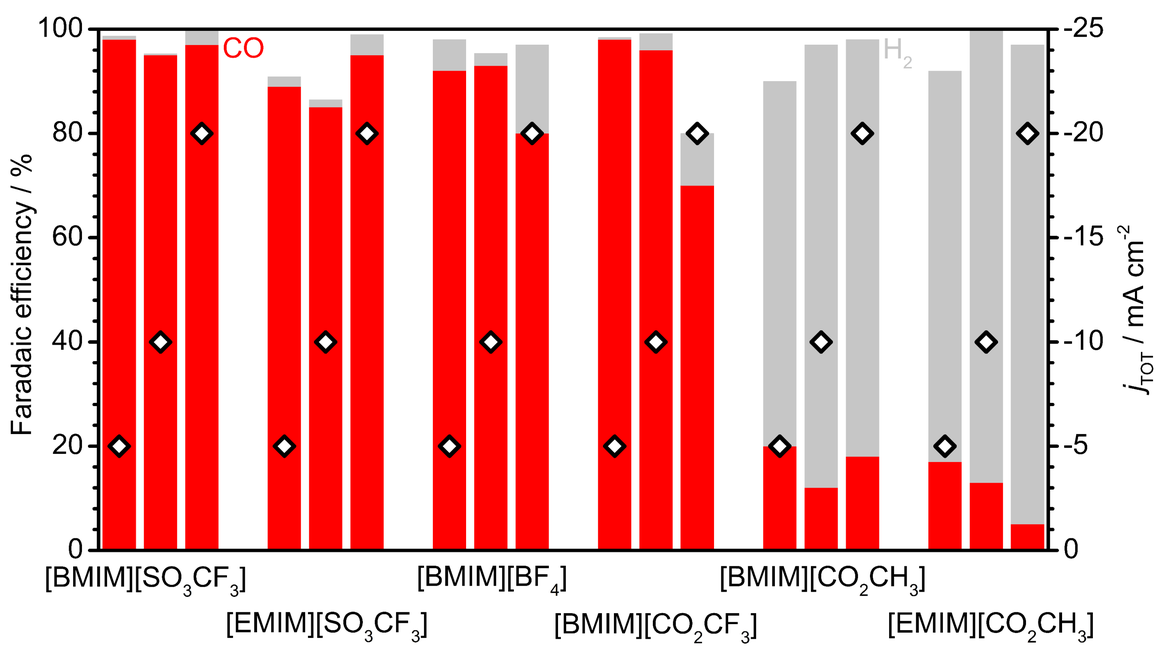
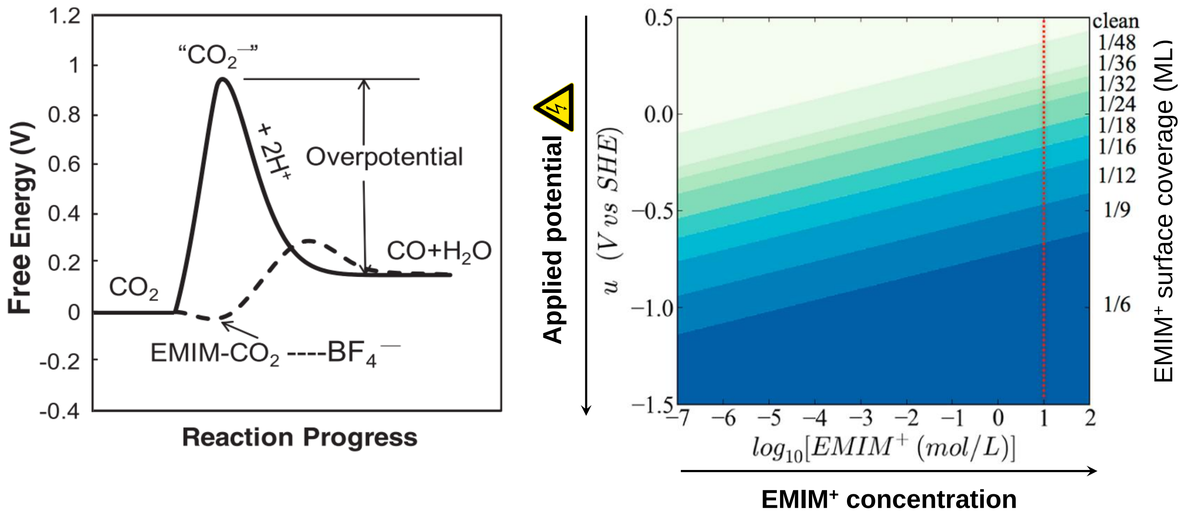
IONIC LIQUIDS EFFECTS IN eCO_2R[1]



Electrochemical CO_2 reduction on polycrystalline silver in imidazolium-based ionic liquids.[1]

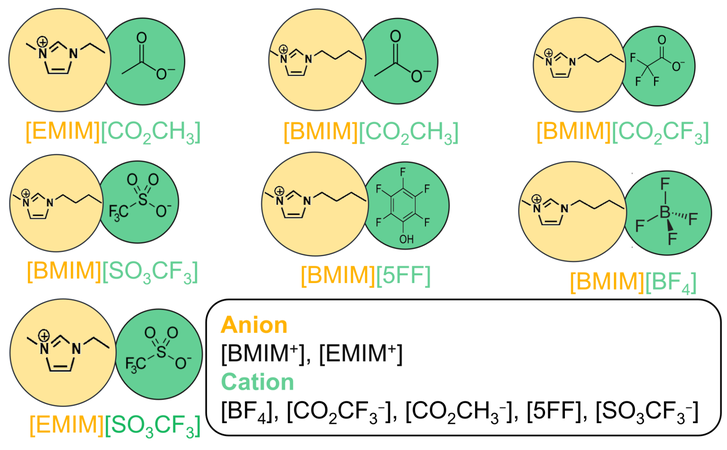
STABILIZATION VS POISONING[2,3,4,5]



Ionic liquids promote CO_2 activation,[2,3,4] yet they can poison the surface at high concentration and negative potential.[5]

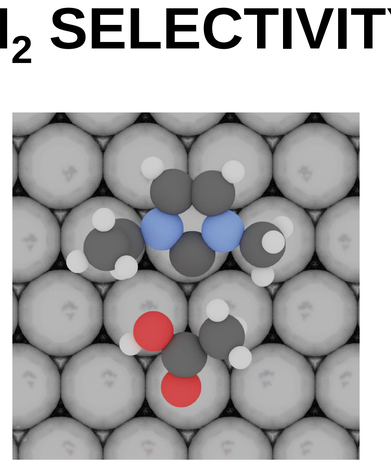
COMPUTATIONAL MODEL[6]

Ionic liquid

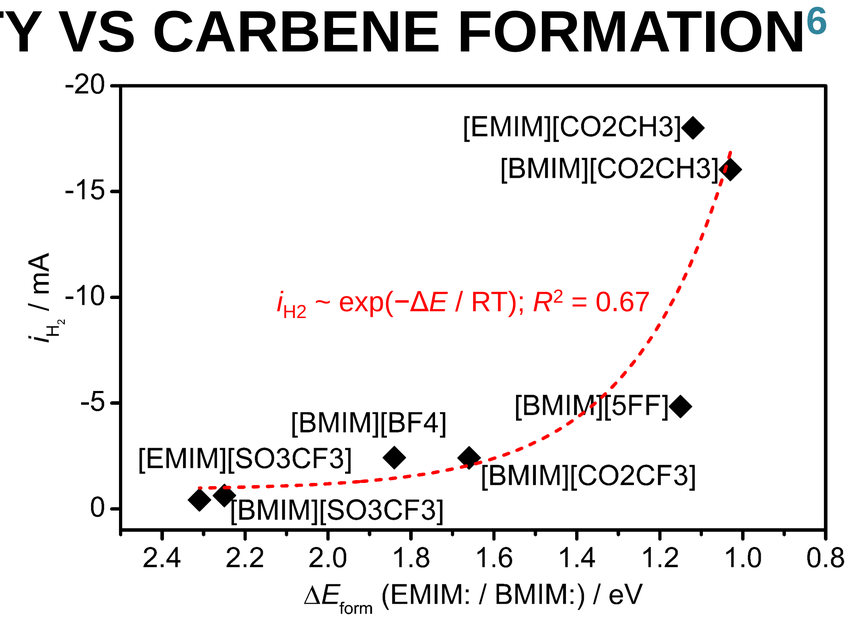


Ag(111) p(3×3)

H_2 SELECTIVITY VS CARBENE FORMATION[6]

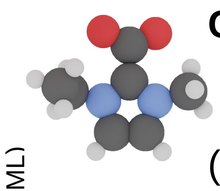


Carbene formation ΔE_{form} (EMIM:)

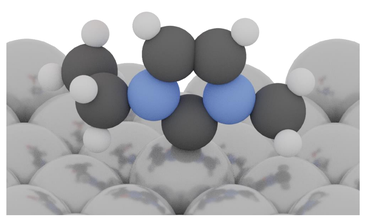


A more favorable carbene formation leads to higher H_2 reaction rates.

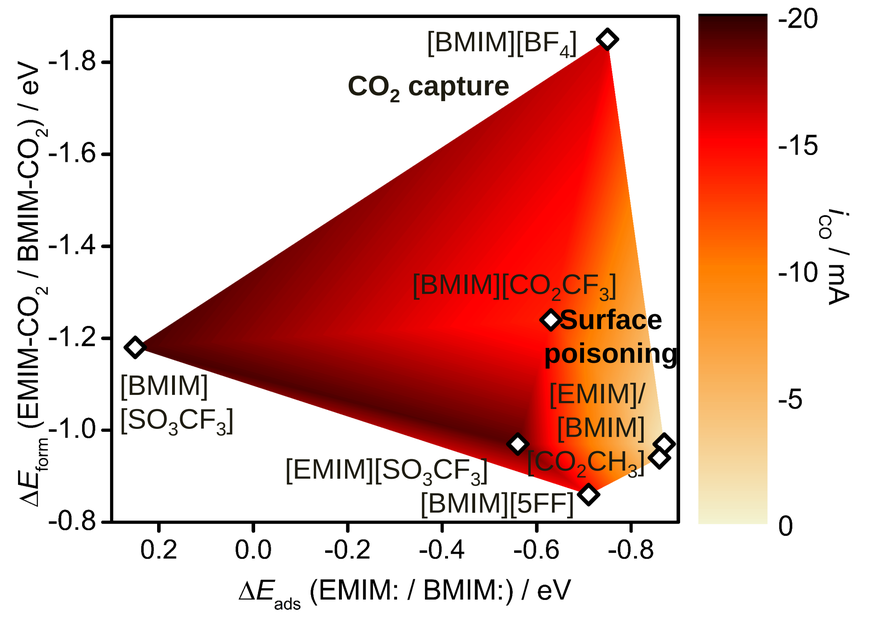
CO SELECTIVITY VS CARBENE FORMATION[6]



Carboxylate formation ΔE_{form} ($EMIM{-}CO_2$)

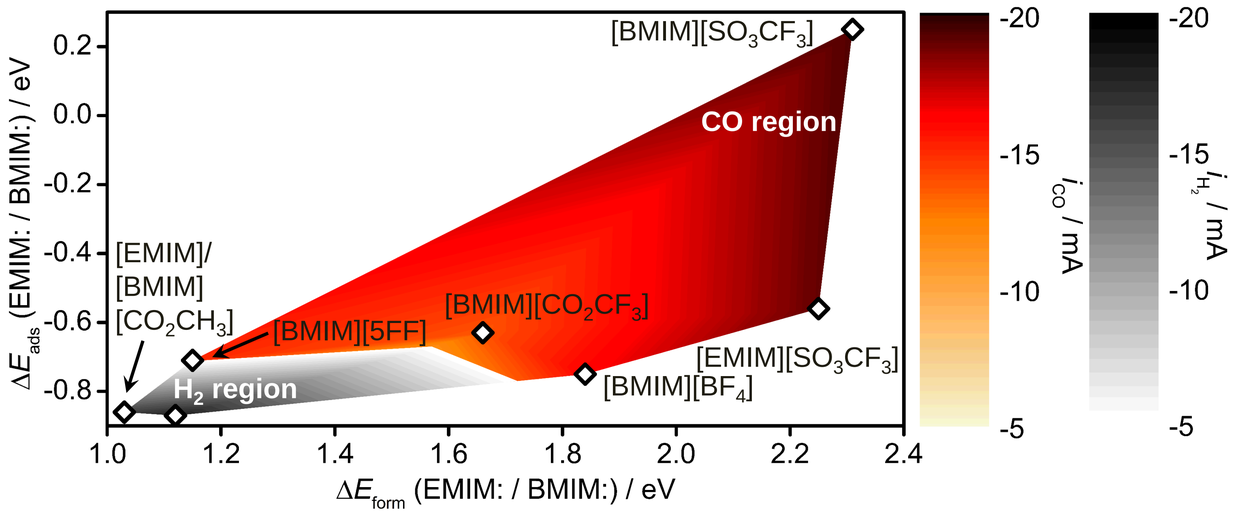


Carbene adsorption ΔE_{ads} (EMIM:)



Once carbenes form, they can adsorb CO_2 or poison the surface, preventing CO_2 reduction to CO.

RATIONAL IDENTIFICATION OF ILs[6]



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