

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Superalkalis as building blocks of noble-metal-free CO₂ activation TIANSHAN ZHAO, JIAN ZHOU, Virginia Commonwealth University, QIAN WANG, peking university, PURU JENA, Virginia Commonwealth University, PROFESSOR JENA LAB TEAM — One of the great challenges to treat greenhouse effect is to convert CO₂ into fuels. The key step for this process requires activation of the CO₂ molecule. Recent experiments have shown that this can be accomplished by reacting CO₂ with noble metal Au. Realizing that the addition of an electron transforms the neutral CO₂ from linear to a bent structure, it was argued that the key parameter that promotes electron transfer from a metal atom to CO₂ depends upon its ionization potential. We note that hetero-atomic clusters known as super-alkalies can be designed such that their ionization potential is smaller than those of alkali atoms. Using first-principles theory we have designed a variety of super-alkali species using different electron counting rules and studied their thermodynamic stability using molecular dynamics simulation. Reaction of these super-alkalies with CO₂ shows that they can be ideal noble-metal free particles for CO₂ activation.

tianshan zhao
Virginia Commonwealth University

Date submitted: 11 Nov 2016

Electronic form version 1.4