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Superalkalis as building blocks of noble-metal-free CO_2 activation

TIANSHAN ZHAO, JIAN ZHOU, Virginia Commonwealth Univ, QIAN WANG, Peking University, PURU JENA, Virginia Commonwealth Univ — One of the great challenges to treat greenhouse effect is to convert CO_2 into fuels. The key step for this process requires activation of the CO_2 molecule. Recent experiments have shown that this can be accomplished by reacting CO_2 with noble metal Au. Realizing that the addition of an electron transforms the neutral CO_2 from linear to a bent structure, it was argued that the key parameter that promotes electron transfer from a metal atom to CO_2 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 CO_2 shows that they can be ideal noble-metal free particles for CO_2 activation.

Tianshan Zhao
Virginia Commonwealth Univ

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