Ab-initio studies on the electronic structure for iridium single-atom catalyst anchored carbon materials toward electrochemical CO_2 reduction to CO

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For alleviating global warming, electrochemical CO_2 reduction reaction (CO_2RR) is one of the remedies to reduce the accumulation of CO_2 because it can be powered by renewable energy and operates at ambient conditions, moreover, the selective products from CO_2 by tailoring the reaction environment. Nevertheless, technologies for CO_2RR have a technical issue due to high overpotential and inevitable HER. Various electrocatalysts have studied to improve the catalytic activity for CO_2RR. Among them, iridium single-atom catalysts have attracted because iridium is beneficial to the adsorption for CO_2 activation and these at the atomic level could provide to increase the metal utilization efficiency. From these results reported previously, we theoretically validated the catalytic activities depend on the electronic structure of iridium single-atom compared to nanoparticles toward CO_2RR to CO and imperative HER by investigating the density of state and the difference of the Gibbs free energy in the reaction process. As a result, iridium single-atom has moderate adsorption/desorption energies with adsorbates for the efficient CO_2RR.