





Hybrid Organic-Inorganic Perovskites: Promising Substrates for Single-Atom Catalysts



Mononuclear metal species are widespread in enzymes and homogeneous catalysts. When such isolated single metal atoms are placed on a solid surface, they can also play an important role in heterogeneous catalysis. In the past few years, great attention has been paid to singleatom catalysts, not only because they can exhibit superior catalytic performance, but also, because they offer a novel way of maximizing the efficiency of utilizing atoms, which is especially desirable in the use of scarce metal elements like platinum. However, single atoms cannot work in isolation but need to be dispersed on suitable substrates.

Qiang Fu and Claudia Draxl have recently demonstrated that hybrid organic-inorganic perovskites - the emerging candidates in solar-cell applications - are highly promising substrates for Pt single atom catalysts. Through systematic first-principles calculations, they found that single Pt atoms are stabilized on such substrates through a synergistic cooperation between covalent bond formation and charge transfer. The generated Pt sites possess excellent catalytic properties in CO oxidation and may be able to play a role in CO2 reduction. This work not only has promising consequences in single-atom catalysis but also sheds light on potential applications of hybrid perovskites as photocatalysts.

Hybrid Organic-Inorganic Perovskites as Promising Substrates for Pt Single-Atom Catalysts

Q. Fu and C. Draxl Physical Review Letters 122 (2019) 046101