## Single-Atom Pd Catalyst Anchored on Zr-based Metal-Organic Polyhedra for Suzuki-Miyaura Cross Coupling Reactions in Aqueous Media

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The challenge for single-atom catalysts in various C-C cross coupling reaction exists in the development of solid supporting materials. It has been desired to find a supporting material designed in molecular level to anchor a single-atom catalyst and provide high degree of dispersion and substrate access in aqueous media. Here, we prepared discrete cages of metal-organic polyhedra anchoring single Pd atom [MOP-BPY(Pd)] and successfully performed a Suzuki-Miyaura cross-coupling reaction with various substrates in aqueous media. It was revealed that each tetrahedral cage of MOP-BPY(Pd) has 4.5 Pd atoms on average and retained its high degree of dispersion up to 3 months in water. The coupling efficiencies of the Suzuki-Miyaura cross-coupling reaction exhibited more than 90.0 % for various substrates we have tested in the aqueous media, which is superior to those of the molecular Pd complex and metal-organic framework (MOF) anchoring Pd atoms. Moreover, MOP-BPY(Pd) was successfully recovered and recycled without performance degradation.