Catalysis at surfaces and interfaces where there exists bi- or multi-component cooperation has been identified as crucial for many processes related to energy and environmental applications. In this talk, I will highlight such cooperative catalysis can be synthetically controlled at the surface and interface of atomically precise nanocrystals, and can play critical roles in maximizing the benefit of oxygen-mediated energy conversion reactions: oxygen reduction reaction (ORR) for fuel cells and oxygen evolution reaction (OER) for water electrolyzer. The first example is M-Pt (M=non-precious metals) core-shell nanocrystals within which desirable/undesirable interfaces between non-precious metal M core and precious metal Pt shell were identified by theoretical calculations and were experimentally balanced by nanocrystal synthesis. The optimized core-shell nanocrystals exhibited favorable interfacial interaction through properly coupled electronic and strain effects, leading to an enhanced electrocatalytic efficiency towards oxygen reduction reaction (ORR).

In the second example, we modulated the interaction of single-site Co, Fe, Ni catalytic centers and inorganic coordination environments in the surface of nanocrystals for electrochemical oxygen evolution reaction (OER). The seamless integration of controlled synthesis of nanocrystals, operando structural/catalytic characterization, and advanced theoretical calculation for oxygen electrocatalyst development will be discussed, which will also be extended to other electrocatalytic processes (e.g. CO₂ reduction and biomass-derived molecule upgrading).