Supporting information for: Density Functional Theory Study on the Adsorption and Decomposition of the Formic Acid Catalyzed by Highly Active Mushroom-like Au@Pd@Pt Tri-Metallic Nanoparticles†

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1 Adsorption of O and OH on the top site in the edge area

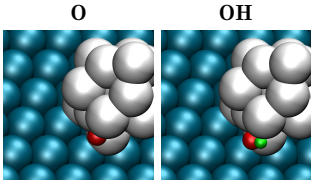

Fig. S1 Optimized structures for O and OH adsorbed on the top site in the edge area of Au@2 ML Pd@0.5 ML Pt NPs.

2 Adsorption of OH in the center area

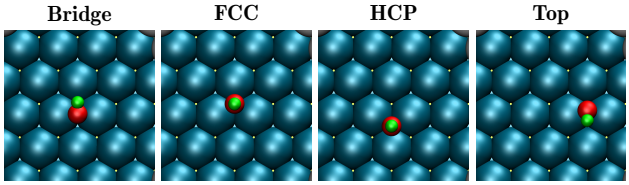

Fig. S2 Optimized structures for OH adsorbed on the center area of Au@2 ML Pd@0.5 ML Pt NPs.

3 Adsorption of HCOO in the edge area

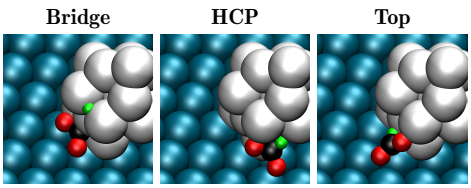

Fig. S3 Optimized structures for HCOO adsorbed on the edge area with fixed adsorption sites of Au@2 ML Pd@0.5 ML Pt NPs.

4 Adsorption of HCOOH in the edge area

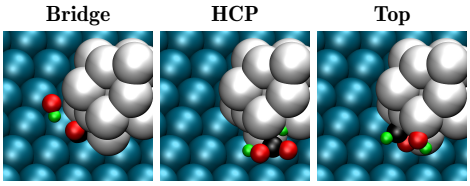

Fig. S4 Optimized structures for HCOOH adsorbed on the edge area with fixed adsorption sites of Au@2 ML Pd@0.5 ML Pt NPs.

5 Adsorption of $COOH_u$ in the edge area

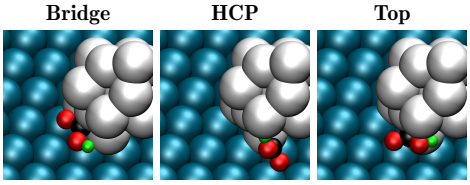

Fig. S5 Optimized structures for $COOH_u$ adsorbed on the edge area with fixed adsorption sites of Au@2 ML Pd@0.5 ML Pt NPs.

6 Adsorption of $COOH_d$ in the edge area

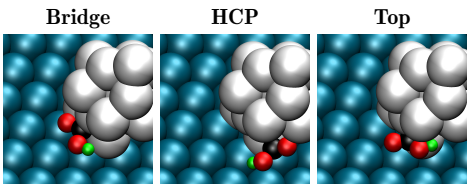

Fig. S6 Optimized structures for $COOH_d$ adsorbed on the edge area with fixed adsorption sites of Au@2 ML Pd@0.5 ML Pt NPs.