Abstract Submitted
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Metal-Organic Chains with Single-Site Pt(II): Insights from first principles simulations[1] DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Creation, stabilization, characterization and control of single atom transition metal sites on surfaces may lead to significant advancement of the next-generation catalyst. Motivated by the experimental results of Skomski eu al. [1], we have performed density functional theory calculations of Pt-dipyridyltetrazine complexes on the reconstructed Au(100) surface. Results of our simulations show that the Pt-dipyridyltetrazine complexes form 1-dimensional chains aligned 45^o with respect to the Au(100) reconstruction row with the molecule-molecule distance of 6.93 Å. More importantly, Bader analysis shows that Pt atoms are cationic with +0.75 charge. This amount of charge is in accord with the charge on Pt in PtO determined by the same analysis indicating that the oxidation states of the Pt atoms in the Pt-dipyridyltetrazine network on the reconstructed Au(100) surface are closer to that of Pt atoms in PtO, which is +2, than in Pt_3O_4 or PtO_3. This result agrees extremely well with experimental XPS data [1]. [1] D. Skomski, C.D. Tempas, K.A. Smith, and S.L. Tait, J. Am. Chem. Soc. 136, 9862 (2014).

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